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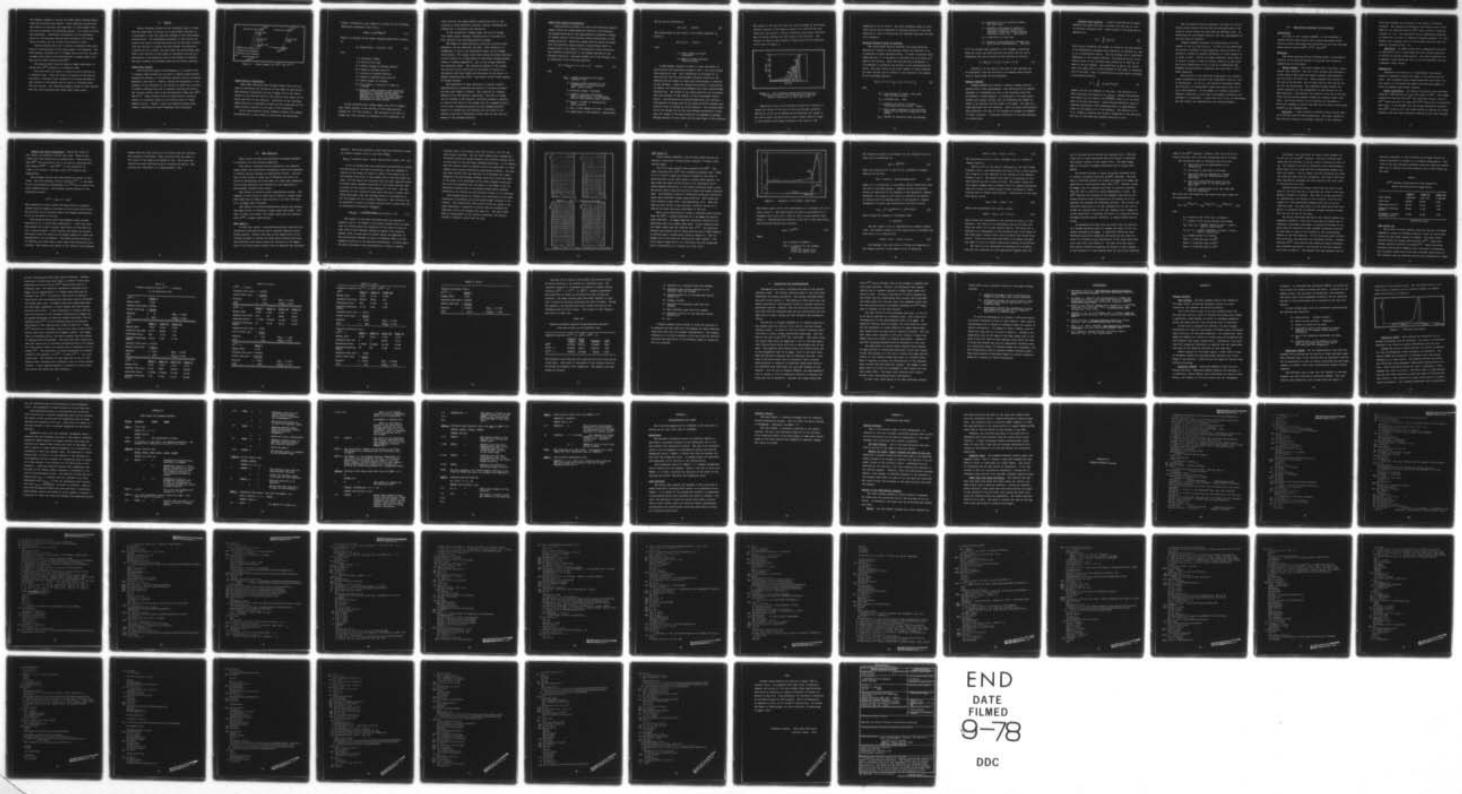

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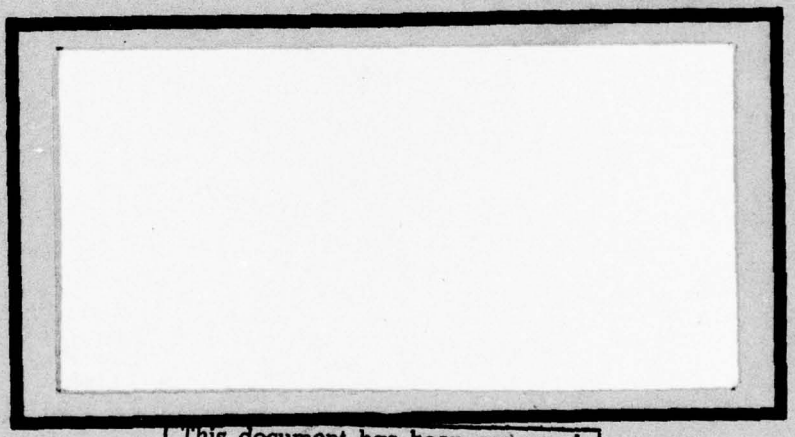

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9 Master's THESIS,

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A COMPUTER CODE TO ANALYZE ALPHA SPECTRA

THESIS

Presented to the Faculty of the School of Engineering
Air Force Institute of Technology
Air University
in Partial Fulfillment of the
Requirements for the Degree of
Master of Science

By

Richard S. Hartley
2nd Lt USAF

Graduate Nuclear Engineering

March 1978

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Preface

This thesis is concerned with the development of a computer code to analyze alpha particle spectra. The reference peak used in the program, obtained from a Po^{210} source, was expressed as a table of values specifying the peak shape channel by channel. The results of the analysis were not within the limits desired but this is thought to be a result of different source thicknesses used.

I would like to extend my sincere gratitude to Dr. George John and Dr. Richard Hagee, my thesis advisors, and to Phil Poirier from whom the original program AUTOFIT was obtained. I would also like to thank Dr. Harold Kirby who enlightened me as to the depth of the problem which was to be undertaken, and Capt Jerome Clifford of the McClellan Laboratory for his interest in the project.

Finally, I would like to thank my wife Cathy, who typed this thesis and whose affection and understanding saw me through this project.

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Abstract

An existing computer code, written to analyze pulse-height spectra from charged particles measured with a mass spectrograph, was modified to analyze pulse-height spectra detected by semiconductor detectors. The program fits the spectra with a reference peak which is expressed as a table of values specifying the peak shape, channel by channel. The modification involved increasing the size of the reference peak to 2048 channels to allow analysis of pulse-height spectra from alpha particles with energies between 4 and 6 MeV. The results of the analysis were strongly dependent upon the reference peak chosen; hence, reference peak selection became the main emphasis of this report. The three reference peaks used were obtained from (1) an empirical function, (2) a single alpha peak obtained from Po^{210}, and (3) an entire spectrum of an isotope to be analyzed. It was desired that the error resulting in determining the area be within three standard deviations of the actual area. The error resulting in each analysis was greater than the prescribed value and was suspected to have occurred because of miscalculation of the reference peak.

A COMPUTER CODE TO ANALYZE ALPHA SPECTRA

I. Introduction

This report presents the results of an investigation of methods for the analysis of pulse-height spectra produced by alpha particles detected by semiconductor detectors. Several goals explored activities of radionuclides, resolution of spectra, the effects of parameters such as source thickness and width of pulse-height interval in obtaining the pulse-height spectra, and various types of algorithms to analyze pulse-height spectra. Major emphasis was placed on obtaining a peak shape representative of a single alpha peak and using this as a reference peak along with existing algorithms to fit alpha spectra.

Background

The general technique of pulse-height analysis consists of determining the area under each peak in the pulse-height spectrum. The area is frequently determined by obtaining an analytical expression which will reproduce the peak shape. The expression is fit to the data by the method of least squares; then numerically integrated to obtain the area. The area represents the total number of particles, with a certain energy, detected by the equipment.

The method of pulse-height analysis has been applied to gamma-ray spectra for quite some time. In gamma-ray spectra, the photopeaks are approximated by Gaussian functions, which can be numerically integrated without difficulty to provide

precise determination of the areas under the photopeaks.

Alpha particles unlike gamma-rays lose energy in small decrements as they collide with the atoms in the detector. As a result of the possibility of small energy losses, the peaks in the pulse-height spectrum are no longer characterized by a pure Gaussian function, but rather by a Gaussian shaped leading edge and an exponential shaped trailing edge. It is difficult to obtain an analytical expression for the resulting peak shape.

Currently, a crude alpha pulse-height analysis technique is being used to analyze alpha spectra obtained from sources, such as Pu^{239} and Pu^{240}. The transition energies of the alpha particles emitted by these isotopes differ by only a few keV; therefore, semiconductor detectors are not able to resolve the peaks resulting from each isotope. However, the contribution from each isotope can be determined by using the sum of the counts from both isotopes along with the known relative amounts of each isotope obtained by mass spectrometry. The limiting factor in this procedure is the determination of the absolute sum of the counts from both isotopes. A summation region approach is currently being used to determine the sum of the counts. This method consists of determining the area under the peak by summing the counts per channel for all channels within a specified region containing the peak. A serious drawback in this method results from information lost in the tails of the peaks. This occurs because of the necessity to specify a region into which the peak must fall. The regions chosen are mutually exclusive; hence, counts found in the long tail extending beyond

the specified region are lost. Greater precision could be obtained if the alpha spectra could be analyzed using a peak shape which would closely approximate the actual alpha peak shape.

Problem Statement

The object of this thesis was to modify an existing computer code and to obtain a peak shape representative of a single alpha peak. This peak shape was then used as a reference peak by the program to analyze the alpha spectra.

Scope

The study was restricted to the use of an existing computer code which was modified to allow analysis of alpha spectra. A reference peak representative of the peaks to be analyzed was required by the program to perform the analysis; hence, a large amount of effort was devoted to obtain a representative alpha peak.

General Approach

The program used in this study was obtained from a program called AUTOFIT, written by J. R. Comfort of Argonne National Laboratory. The major modification was to increase the allowed number of channels in the reference peak from 40 channels to 2048 channels. After modification, the program was renamed ALPHAFIT and was tested to determine its peak fitting capability.

An analytical function was used to generate emulated pulse-height spectra. For simplicity, a Gaussian pulse-height distribution was used. Studies were made of the capabilities of

the computer program to resolve two peaks whose relative amplitudes and positions were varied. Other variables studied were the effects of resolution and magnitude of pulse-height interval used to generate the simulated spectra. Two series of tests were performed. Statistical fluctuations of the individual points in the simulated spectra were included in the second series of tests, but not in the first series of tests.

Several methods were used to obtain a reference peak which would be representative of the alpha peaks to be analyzed. The first method, developed by P. De Regge (Ref 2:271-272), allowed a single alpha peak to be extracted from a complex alpha spectrum such as that obtained from Am^{241}.

The second method involved using a single alpha peak obtained from Po^{210} directly as a reference peak.

The last method was based on using an entire spectrum as a reference peak. Since the types of isotopes in the spectra are known, a reference peak composed of an entire spectrum of each isotope in the spectra can be used as a reference peak for that isotope. The resulting analysis should be more precise and less time-consuming than using single alpha peaks.

II. Theory

Before becoming involved in the techniques used to determine the area under the peaks in a pulse-height spectrum, it is important to know the cause and meaning of the pulse-height distributions. The information presented in this section describes the source of alpha particles and the way they interact with the detector to produce the pulse-height distributions. A method on how to relate the area under the pulse-height spectrum to the activity of the source is described followed by a description of the algorithm used by the program to minimize the error between the reference peak and the actual spectrum.

Alpha Decay Process

The motivation behind the development of a computer code to analyze alpha spectra was the need to analyze alpha spectra produced by mixtures of low-activity sources, such as plutonium, americium, and curium. However, during the development of the program, it was necessary to use sources of sufficient activity to reduce counting times and to increase counting statistics. The two main sources used in the developmental stage were Am^{241} and Po^{210}. These isotopes decay by alpha particle emission either to the ground states or the excited states of their daughter nuclei. Figure 1 shows the simplified alpha decay scheme, describing the major branchings (Ref 4:435,403).

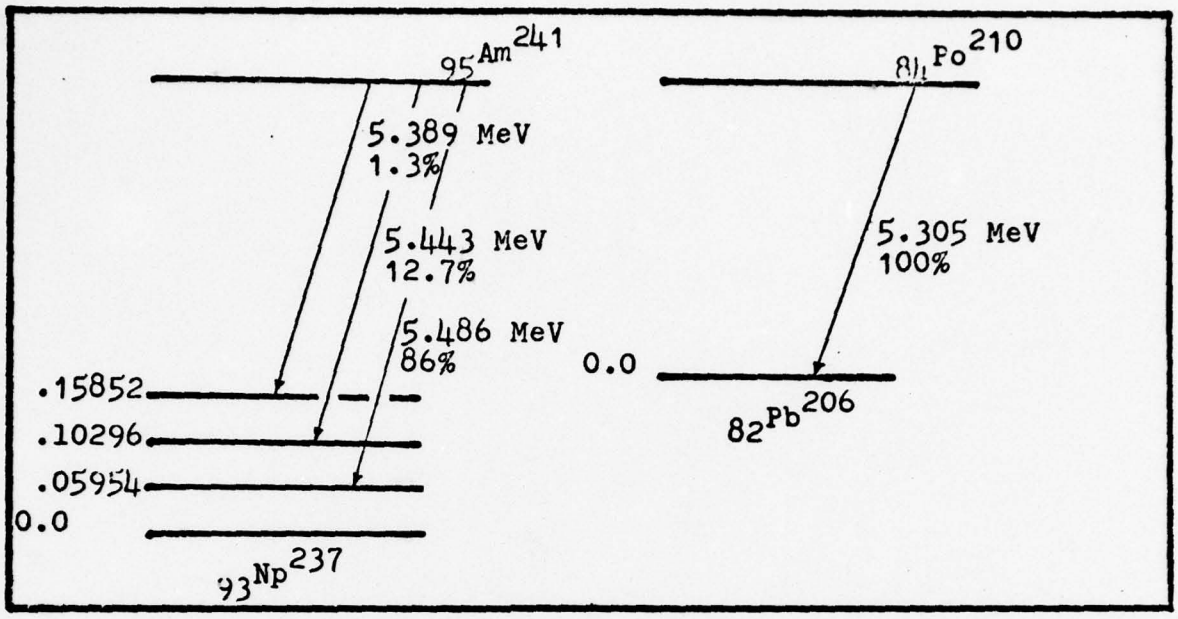

Figure 1. Decay Schemes for Am^{241} and Po^{210}

Alpha Particle Interaction

When alpha particles pass through matter, they lose energy by excitation and ionization of the atoms of that matter. The mechanism responsible for this energy loss is the interaction of the Coulomb fields of the particle with those of the bound electrons in the material. Deflection of the incoming alpha particles is negligible because of the large mass of the alpha particle relative to the mass of the electrons.

As an alpha particle passes through a medium, the energy dE transferred to that medium by ionization and excitation

along a differential path length dx is given by the following theoretical expression (Ref 5:3-4):

$$-dE/dx = 4\pi e^4 z^2 NB/mv^2 \qquad (1)$$

where B is defined as the atomic stopping number and is given by

$$B = Z[\ln(2mv^2/I) - \ln(1-\beta^2) - \beta^2] \qquad (2)$$

with

e = electronic charge

m = electron rest mass

E = kinetic energy of primary particle

ze = charge of primary particle

v = velocity of primary particle

N = number of absorber atoms per cm^3

Z = atomic number of absorber

β = v/c, where c = velocity of light in a vacuum

I = geometric-mean ionization and excitation potential of absorbing atoms; cannot be calculated accurately and generally regarded as a constant for each element. The value of I must be experimentally determined for each element.

In the nonrelativistic energy range, the rate of energy loss -dE/dx depends on the velocity of the alpha particle through the $1/v^2$ term in Eq(1). The increase in the rate of energy loss with decrease in velocity is to be expected. At

lower velocity the alpha particle spends more time in the vicinity of bound absorber electrons, thereby increasing the probability of ionization and excitation.

In the relativistic energy range, the rate of energy loss -dE/dx passes through a minimum which is followed by a slow increase with increasing particle energy.

The ranges of alpha particles, which are initially monoenergetic, are not precisely the same. This variation, or straggling, is due to the statistical nature of the energy-loss process. The energy losses which bring the alpha particles to rest consist of a large number of individual energy-transfer events of varying magnitudes. Most of the energy transfers are relatively small. The statistical nature of the energy-loss process allows variations in the number of events occurring per unit path length and variations in the amount of energy transferred per event. Few events involve large amounts of energy transfer.

The absorption of alpha particles is usually studied experimentally by measuring the number of ion pairs produced per unit path length of travel. This quantity is commonly referred to as the specific ionization. The rate of energy loss is related to the specific ionization through a quantity w, which is the ratio of the energy lost by a charged particle to the total ionization produced by that charged particle. Values of w depend upon the material and the state of the material with which interaction occurs, and the type and the energy of the incident particle.

Alpha Pulse Height Distributions

Alpha particles incident on solid state detectors deposit energy within the charge-depletion region of the detectors. The energy deposited by the alpha particles produces a number of charge carriers (electron-hole pairs) proportional to the energy deposited. These free charge carriers which are swept from the depletion region produce a pulse height which is proportional to the number of electron-hole pairs collected, and therefore proportional to the energy deposited by the incident radiation. The pulse height out of the detector can be expressed by the following equation:

$$ph = [(E_{dep}/w) \times e \times \gamma] \times 1/C \quad \text{(volts)} \qquad (3)$$

with

E_{dep} = energy deposited by the alpha particle (eV)

w = average energy required for the production of an electron-hole pair (eV/e-h pair)

e = electron charge (coulombs)

γ = charge collection efficiency. This is essentially 1 in detectors made of high quality single crystals

$N = E_{dep}/w$ = number of electron-hole pairs produced

$q = Ne\gamma$ = total charge collected (coulombs)

C = capacitance of the detector (picofarads)

Eq (3) can be rewritten as

$$ph = q/C \quad \text{(volts)} \tag{4}$$

The pulse-height at the output of the linear amplifier is given by

$$PH = q \times G \quad \text{(volts)} \tag{5}$$

with

q = total charge collected (coulombs)

G = gain of linear amplifier (volts/coulomb)

A multichannel analyzer is used to count the number of times pulses with amplitudes between h and h + Δh occur during the acquisition time. This information is displayed on an oscilloscope with the pulse-height intervals plotted on the abscissa and the number of times each pulse-height is observed on the ordinate. Since the energy-loss process is statistical in nature, the resulting pulse-heights will form a pulse-height distribution. The energy of the alpha particles are associated with the location of the maximum in the pulse-height distribution. The distribution of pulse-heights does not reflect a distribution of energy lost by the alpha particles because each particle loses an energy E_o in the detector. The tailing effect on the low energy side of the pulse-height distribution occurs when the energy of the alpha particles is degraded by passage through material in the source and the dead layer of the detector.

The length of the path and thus the loss in energy by each alpha particle depends on the angle at which it is emitted from the source and the extent to which it deviates from normal incidence when it passes through the dead layer of the detector. The effects of various path lengths of alpha particles through gold can be seen in Figure 2.

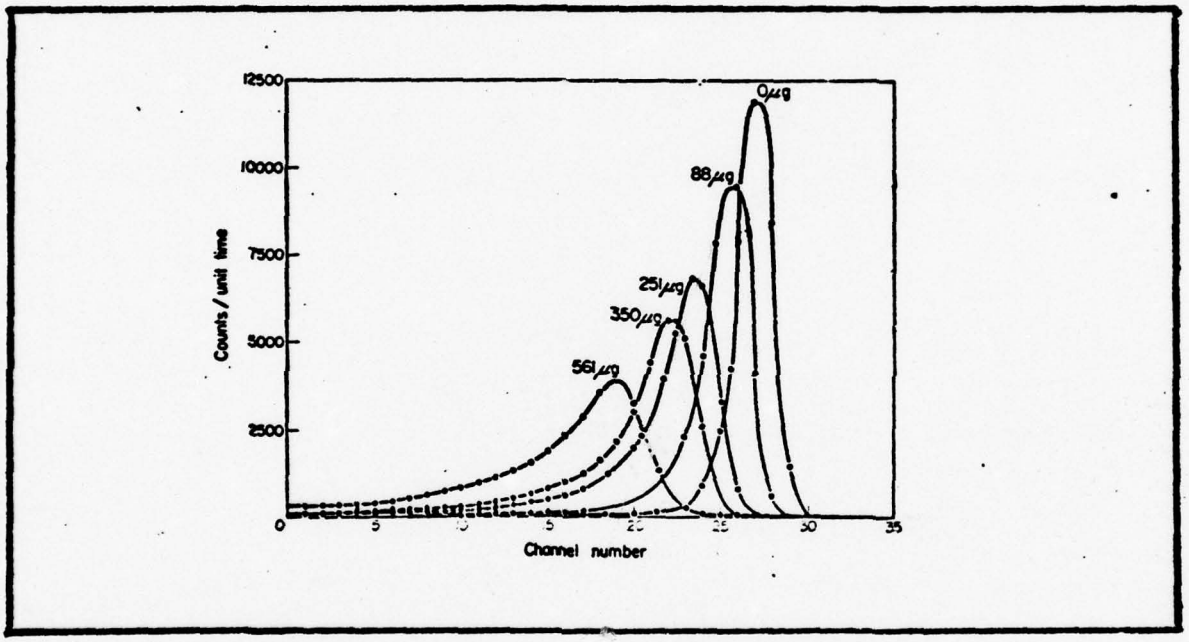

Figure 2. The α-particle Energy Distribution for a Thin Source of Pu^{239} After Transmission Through Various Thicknesses of Gold (Ref 6:108)

Electronic noise in the detection system will further increase the spread of the peak in the pulse-height spectrum. Electronic noise can be determined by measuring the spread in the pulse-height spectrum from a pulser signal which is equal to the average pulse-height produced at the input to the

preamplifier by the source. The peak spreading caused by electronic noise can be neglected in spectrum analysis if the same equipment is used to obtain both the reference peak and the data to be analyzed.

Relating Observed Counts To Activity

The pulse-height spectra obtained from alpha particles emitted by isotopes of the actinide series are expected to be a composite of peaks described above. In order to analyze these alpha spectra, it is necessary to determine the area under each peak in the spectra. After the area has been determined, it is necessary to determine the activity of the contributing isotopes. The area, which is the total number of counts observed for each isotope, can be related to the activity of the sample by the following equation:

$$N_t/t_c = A \times G \times f_{ss} \times f_w \times \delta \times f_t \times f_\alpha \qquad (6)$$

with

N_t = total number of counts = the total area for each isotope

t_c = counting time (sec)

A = activity of source in nuclear transformations per second (ntps)

G = solid angle subtended by the sensitive region of the detector relative to the source

f_{ss} = scatter of radiation from surroundings

f_w = absorption by air, detector window, and dead layer

δ = intrinsic efficiency of detector = fraction of particles which enter sensitive volume and produce a pulse, assuming no dead time (#cnts/#α's)

f_t = correction for dead time

f_α = number of alpha particles observed for each nuclear transformation (#α's/nt)

If it is assumed that equipment is not changed, scattering does not occur, and dead time does not exist, Eq (6) can be simplified and can be solved for the activity as follows:

$$A = (N_t/t_c) \times (1/f_\alpha) \times (1/G) \times (1/\delta) \qquad (7)$$

Therefore, if the area of each peak in the spectrum can be calculated, then the activity of an unknown sample giving rise to those peaks can be determined.

Program ALPHAFIT

Program AUTOFIT was written to analyze charged particle spectra from a mass spectrograph. The modifications on AUTOFIT included (1) increasing the size of the reference peak from 40 channels to 2048 channels, (2) disposing of the peak search routine and Q-value options, and (3) decreasing the number of peaks to be analyzed from 200 peaks to 20 peaks. The peak fitting algorithms were not modified. After the above modifications were performed, the name of the program was changed to ALPHAFIT to avoid confusion. A detailed description of the peak analysis is listed below.

Detailed Peak Analysis. A complex spectrum can be represented by an array [E] which is formed from the sum of a set of resolved components Z(x). Each element of the array can be expressed as

$$E_i = \sum_{l=1}^{L} a_l Z_i(x_l) \qquad (8)$$

where $Z_i(x_l)$ designates the number of counts in the ith channel of an unnormalized reference peak located at an abscissa x_l, and a_l is a normalization factor. The sum extends over L individual components in the complex spectrum. The quantity $Z_i(x_l)$ is defined as zero if the reference peak located at x_l does not extend to the ith channel. The quantities x_l and a_l are varied until the array [E] is closely matched to the array of ordinates [Y] of the data. This is quantitatively accomplished by forming a chi-squared function

$$F = \sum_{i=1}^{N} (Y_i - E_i)^2 / (\delta Y_i)^2 \qquad (9)$$

summed over all the channels of the data. The function F is then minimized with respect to a_l and x_l. During minimization, the weights δY_i are taken to be $\sqrt{Y_i + 10}$, where Y_i is the ordinate of the ith data point. Since Poisson Statistics apply in counting experiments, this weighting factor is approximately equal to the square root of the variance. The addition of 10 to Y_i slightly increases the relative weighting of the data near the tops of the peaks and prevents division by zero.

The chi-squared function represents the ratic of the observed spread between the data and the reference peak to the expected spread between the data and the reference peak. By minimizing the chi-squared function, the best approximation to the real data is obtained.

Program ALPHAFIT separates the minimization of F with respect to the a_l's and the x_l's. If the x_l's are known from the initial estimates of peak positions, the a_l's can be obtained by setting the partial derivative of F with respect to a_l equal to zero. The set of linear equations, which need to be solved in order to find the correct value of a_l and which will allow minimization of F, is set up in Subroutine FCN. Standard matrix-inversion techniques are then used to solve these equations.

The position of the peaks are established by a variable metric minimization procedure (Ref 7:ANL-5990) coded in a set of subroutines. As the x_l's are varied by Subroutine SHIFT, the function F is recalculated (each time with a best set of a_l's) and inspected. If the change in F between successive complete iterations is less than a convergence criterion, the procedure is terminated. A final best set of a_l's is calculated, and the results are transmitted to the calling program.

III. Experimental Equipment and Procedures

Introduction

In order to test Program ALPHAFIT, it was necessary to obtain selected alpha spectra with certain parameters fixed. For this reason experiments were performed on site with existing alpha sources such as Am^{241}, Po^{210}, and Pu^{240}.

Equipment

The alpha spectroscopy was performed using a semiconductor detector in an evacuated chamber to maximize the resolution capabilities of the system.

Vacuum Chamber. The vacuum chamber was a two-piece, cylindrical steel canister. The top of the canister was fastened to a wood support which held the chamber assembly approximately one foot above the table top. Three openings were located in the top of the canister, two of which were an inlet and an outlet for the vacuum pump. The remaining opening allowed the direct connection of the preamplifier to the detector by two BNC connectors. The detector was mounted to the top of the canister and was facing downward toward the moveable source platform. The bottom portion of the canister was removeable to allow the changing of sources and was held in place by the vacuum created by the roughing pump.

Detectors. A high resolution detector with an active area of 25 mm^2 was used for data acquisition. The small surface of this detector required a necessary increase in the counting

times and required the reduction of the source to detector distance. The resolution obtained by this detector was 18 keV FWHM for the 5.486 MeV peak of Am^{241} with a source to detector distance of 1 cm. The resolution was not appreciably affected by variations in source to detector distances between 1 to 3 cm; however, the counting times for the sources used were much too long for distances above 1 cm.

Amplifiers. An ORTEC, Model 142-B, preamplifier was used in conjunction with a linear amplifier and a biased amplifier to obtain the desired alpha spectra. The linear amplifier was a Tennelec, Model TC203 BLR, and the biased amplifier used was a Tennelec, Model TC250A.

Experimental

Throughout the entire set of experiments, the maximum amount of separation between the peaks of the spectra was desired. This required using a biased amplifier which would cut out signals of low energy and expand the remaining signals to allow the maximum peak spread possible.

Energy Calibration. All energy calibrations were performed using the 5.486 MeV and the 5.443 MeV peaks of Am^{241}. The energy calibration obtained from Am^{241} was used when sources, such as Po^{210} (which has only one peak) and Pu^{240} (which had low activity), were used. It was assumed that the energy calibration obtained from Am^{241} could be used with other sources as long as the linear amplifier and the biased amplifier remained at the same settings.

Sources and Source Preparation. During the course of this study, six different sources were used. Three of the sources had been prepared at an earlier date. These sources were Am^{241} with an activity of 0.1 μCi and two plutonium samples labeled Pu^{240} - 1 and Pu^{240} - 2 with activities of 2.583×10^5 α's/min ± 1.5% and 2.598×10^4 α's/min ± 2%, respectively.

Two polonium sources were made during the course of this study. The first polonium source, labeled Po^{210} - 1, was made by the electrochemical displacement of Po^{210} onto a silver disk from a RaDEF solution. The plating occurred because of the following reaction:

$$Po^{+++} + 3Ag \rightarrow Po + 3Ag^{+}$$

This disposition occurs without the application of external current when the RaDEF is dissolved in nitric acid (Ref 6:100). The activity of this polonium source was roughly approximated to be of the order of 0.03 μCi.

The second polonium source was prepared using a method described by H. W. Kirby (Ref 3:2043-2047). A half inch platinum square was rinsed in water; then fired to a red heat for ten to twenty seconds. After cooling, the square was sprayed with Krylon with the center of the square masked by a brass rod approximately 7 mm in diameter. The RaDEF solution which was in 0.8N HNO_3 was dried under a heat lamp; then redissolved with 1.5N HCL. The solution was placed in the center of the platinum

square which was then placed on a hot plate until the solution was completely evaporated. Then, 3N acetic acid was added to the center of the square and allowed to dry. The source was rinsed with water and then acetone to remove the Krylon. The activity was calculated to be approximately 1 μCi.

IV. Data Reduction

Three series of tests were performed on Program ALPHAFIT to determine its peak fitting capability.

Test Series I involved spectra composed of two Gaussian shaped peaks with statistical fluctuations which were generated to emulate spectra obtained by experimental methods. The purpose of this series of tests was to determine the error involved in determining the areas under the peaks when parameters such as peak amplitude, peak separation, and magnitudes of pulse-height intervals were varied.

Test Series II involved actual experimental spectra. The emphasis in this series of tests was to extract a single alpha peak shape from a complex alpha spectra by a method developed by P. De Regge (Ref 2:269-280).

Test Series III involved experimental spectra and emphasis was again placed on obtaining a single alpha peak shape. However, in this test series, the single alpha peak was obtained from Po^{210}, a single alpha emitter.

Test Series I

In this test series, a Gaussian pulse-height spectrum with statistical fluctuations was used to generate emulated pulse-height spectra. Studies were made of the capabilities of the computer program to resolve two peaks whose relative positions and amplitudes were varied along with variation in the magnitude of the pulse-height interval used to generate the simulated

spectra. The error involved in each study was reported in terms of relative percent error in peak area (RPE_A).

$$RPE_A = \left| \text{(computed area - actual area)/actual area} \right| \times 100 \quad (10)$$

If it is assumed that the statistical fluctuations in counts are described by a Poisson distribution, then the standard deviation in the number of counts is equal to the square root of the average total count or the square root of the area under the peak. In this report the criterion that the area computed should be within three standard deviations of the actual area was used in order for the results of the analysis to be valid. The satisfaction of this criterion would allow the user to state, with 99.7% confidence, that the limiting factor in the analysis is not the program but the counting statistics. This criterion can be expressed in terms of relative percent error in peak area due to statistical fluctuations ($RPE_{\sqrt{A}}$).

$$RPE_{\sqrt{A}} = (3\sqrt{\text{actual area}}/\text{actual area}) \times 100 \quad (11)$$

The results of the tests described above are plotted in Figures 4 and 5. In Figure 4 the relative percent error in peak area is plotted versus the separation of the peaks in units of full width at half maximum, whereas in Figure 5 the relative percent error in peak area is plotted versus the magnitude of the pulse-height interval in units of σ/channel where σ is the standard deviation of the Gaussian distribution. In each figure the error resulting in the determination of Peak 2 is being

plotted, Peak 2 (P2) being to the left of Peak 1 (P1) in the pulse-height spectrum. The two heavy dashed lines running horizontally across each graph signifies the relative percent error in peak area for one and three standard deviations. It is assumed that the results shown in Figures 4 and 5 are applicable to other complex alpha spectra obtained by experimental methods. The user must make certain that the spectrum to be analyzed has a peak separation and pulse-height interval which will allow the areas of the peaks to be determined within three standard deviations. This will not guarantee that the areas of the peaks in the experimental spectrum will be determined within three standard deviations, but affords the best possible chance of it occurring.

The program appears to operate more efficiently as the peak separation is decreased and as the pulse-height interval is increased. This unrealistic result which occurs for peaks of unequal amplitude is suspected to result from the minimization algorithm used by the program (see page 15). The exact cause was not investigated in this report; therefore, the results plotted in Figures 4 and 5 will be used.

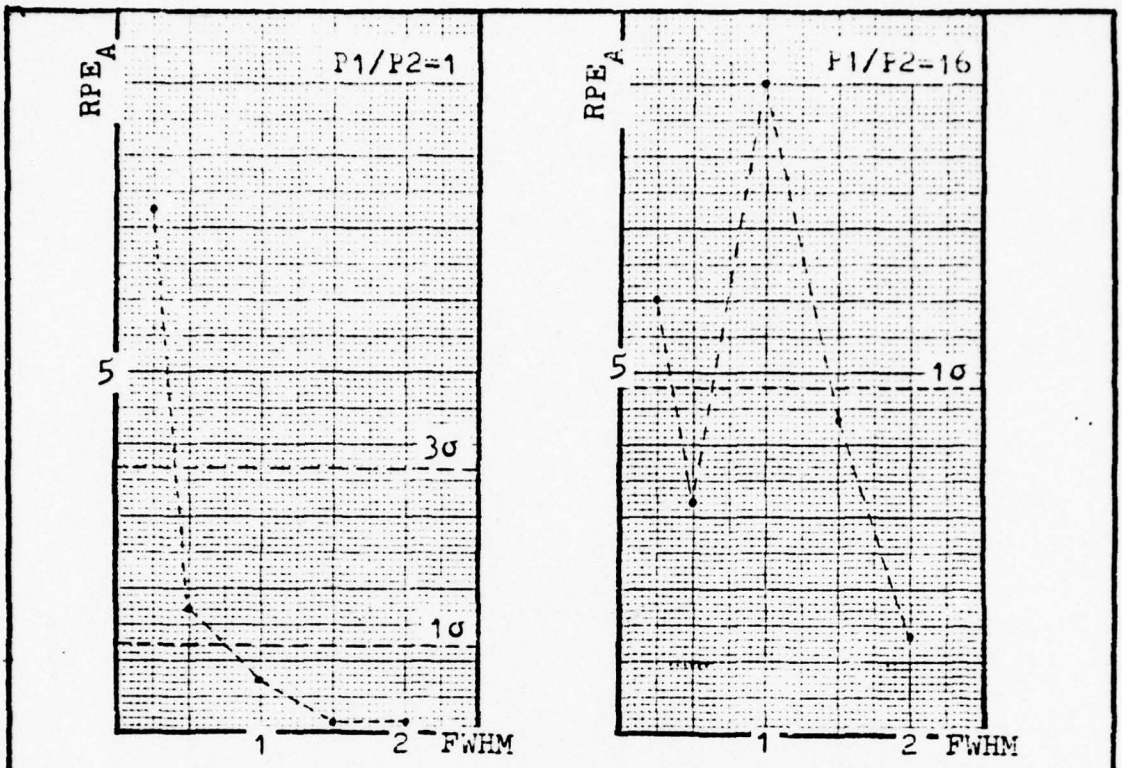

Figure 4. RPE$_A$ vs. Separation in FWHM

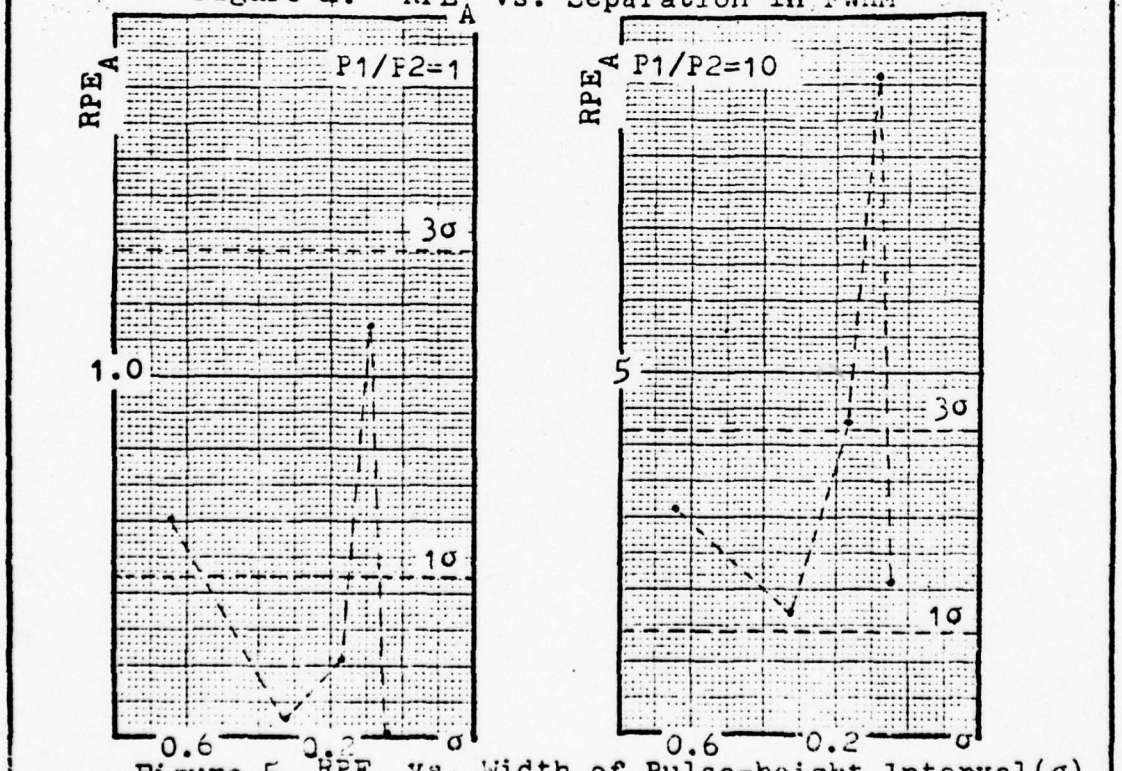

Figure 5. RPE$_A$ vs. Width of Pulse-height Interval(σ)

Test Series II

After Program ALPHAFIT's peak fitting capability was determined using peaks of known areas, analysis of actual alpha spectra began.

The first alpha spectra were obtained from Am^{241}. The peaks resulting from Am^{241} had a separation greater than 1 FWHM. If it is valid to apply the results obtained in the limit of precision test on the ideal peaks to actual alpha spectra, the area under the peaks should be able to be calculated within three standard deviations if the correct reference peak is used. The problem which resulted was how to obtain the proper reference peak. All available sources of sufficient activities emitted at least three different energy alpha particles. Each alpha particle creates a peak with a long exponential tail. When more than one peak exists in the spectrum, confusion exists as to exactly how much each peak contributes to the tail.

Since it was impossible to obtain a reference peak directly from the Am^{241}, a method developed by P. De Regge was applied (Ref 2:269-280). De Regge based his empirical relation on observations made on a single alpha peak. It was suspected that the single alpha peak was obtained from Po^{210}. The empirical relation was derived from an alpha peak plotted in 2048 channels on semilog paper (schematically shown in Figure 6). The low energy side of the peak was divided into three regions. The first region ranges from 0 to 3 MeV below the peak energy and can be represented by a constant flat line (a-b).

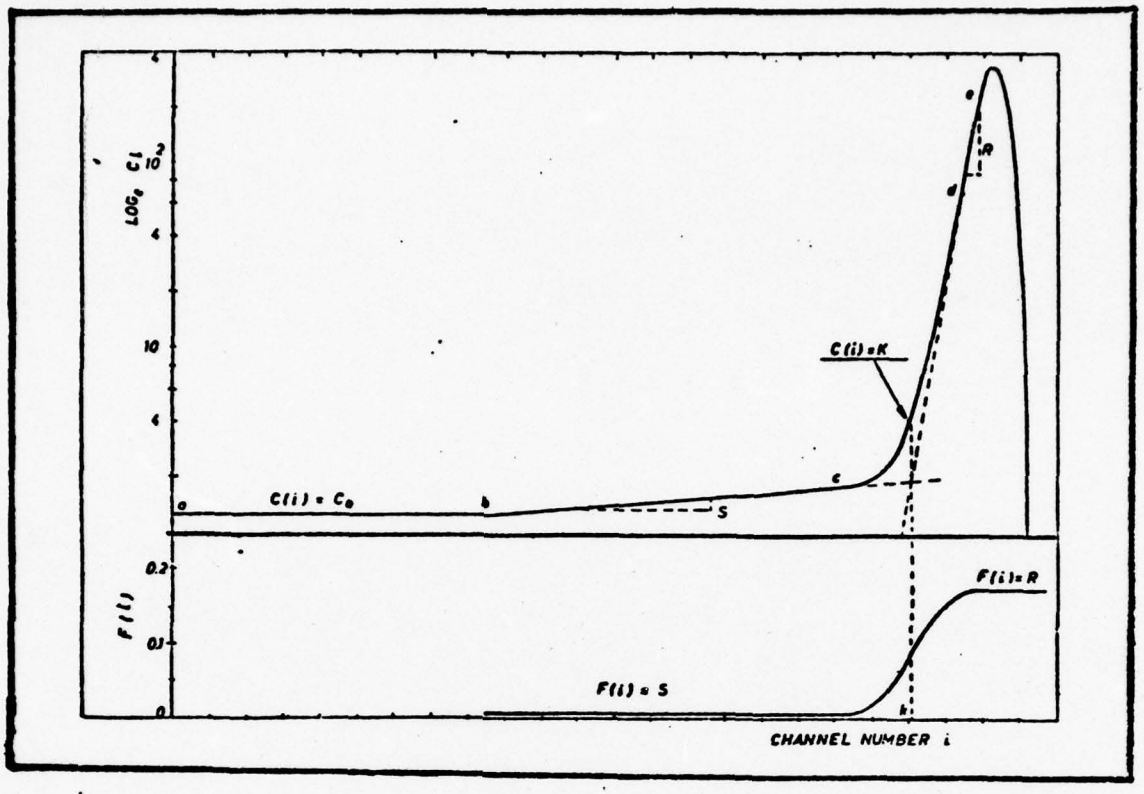

Figure 6. Schematic of De Regge's Alpha Peak

The second region can be best represented by a straight line (b-c) with a slope S. The third region can best be represented by a straight line (d-e) with a slope R, which is much greater than slope S. Considering the spectrum to the left of the peak value, the following equation was proposed:

$$C_{i+1} = C_i e^{F(i)} \tag{12}$$

where

C_i = content of channel i

F(i) = a function of the channel number i
S for the region (b-c)
R for the region (d-e)

The transition region (c→d) between the two straight line sections can be represented by

$$C(i) = e^{\int F(i)di} \tag{13}$$

where the function F(i) is best fit by a hyperbolic tangent function of the form

$$F(i) = (R+S/2) + [(R-S/2)\tanh\alpha(i-k)] \tag{14}$$

where α is a coefficient to accomodate various transitions from the tail to the peak regions. Negative as well as positive values are required for the argument of the hyperbolic tangent; therefore, the origin of the i-axis is shifted by an amount k to coincide with the bending point of the hyperbolic tangent. Integration of Eq(14) and substitution into Eq(13) yields

$$C(i) = 2^{1/z}\, K[e^{zR(i-k)} + e^{zS(i-k)}]^{1/z} \tag{15}$$

with K being the constant of integration and

$$z = 2\alpha/(R-S)$$

The tail region (b→c) is characterized by channel numbers $i \ll k$. The channel contents in this region yield a straight line with slope S on a semilog plot.

$$\ln C(i) = \ln K - 1/z\ln 2 + S(i-k) \tag{16}$$

The straight line with slope R, fitting the logarithm of the channel contents in the region (d→e), is given by

$$\ln C(i) = \ln K - 1/z\ln 2 + R(i-k) \qquad (17)$$

The intersection point of these straight lines is located at channel number k.

Eq(15) is fit to the data by obtaining C_o, the tail height between a and b, and determining the slope R from a least squares fit of Eq(17) to the logarithm of the contents of the channels between d and e. The slope S was found to be constant in several spectra and had a value of 0.004. The point b where the tail region changes from a constant value to a gently increasing curve was chosen as channel number (k-700) according to observations made on several alpha spectra. Substitution of the above into Eq(16) yields

$$\ln C_o = \ln K - 1/z\ln 2 - 2.8 \qquad (18)$$

which, when substituted into Eq(17), yields

$$\ln C(i) = \ln C_o + 2.8 + R(i-k) \qquad (19)$$

which allows the calculation of the location of point k on the abscissa. The value of z is determined only by the ratio α/R since the value of S is much smaller than R. The ratio α/R is expected to be independent of the resolution and of the shape of the alpha peaks, because both α and R increase with better resolution. Values for $2\alpha/R$ have been found to be nearly constant and equal to 0.59 for typical resolutions between 20 and 80 keV.

The value of K is calculated by replacing C(i) in Eq(15) with the real contents of a few undisturbed channels near the

top of the peak and by solving the equation for K. The mean value of K is then substituted back into Eq(15) to calculate the channel contents in the region (b→e). The high energy edge of the peak is assumed undisturbed and is simply integrated.

An attempt was made to apply the method described above to obtain a reference peak from an Am^{241} spectrum. This was done to determine whether the method developed by De Regge was applicable to alpha spectra other than Po^{210}. However, unlike De Regge, only 512 channels were used to store the spectrum. This was done to allow for easier manipulation of data. The Am^{241} spectrum was obtained in 512 channels with the aid of a biased amplifier which eliminated the low energy end of the spectrum and expanded the remaining spectrum. This allowed the prominent alpha peaks to be well separated but at the cost of losing the constant part of the tail (Region (a→b), Figure 6). It was impossible to determine the value of k using the method De Regge described above; therefore, a simpler method was devised.

An assumption was made from the outset that the addition of a biased amplifier would not change the values of the constants obtained by De Regge. A simplified method was then developed using this assumption and using the fact that the point k is located at the intersection of the lines drawn from (b→c) and (e→d) (see Figure 6). The line (e→d) and slope R were easily obtained by applying the method of least squares to the contents of a few channels near the top of the 5.486 MeV

peak of the Am^{241} spectrum. However, line (b→c) was not so easily obtained, and a few more assumptions had to be made.

The assumptions made in obtaining line (b→c) were

a) each tail could be approximated by an exponential,

b) the slope of each tail is the same,

c) the total tail is composed of a linear combination of the contribution from each peak,

d) each peak contributed an amount to the tail proportional to the area under its peak, and

e) the tail contributions above the 5.486 MeV peak are negligible.

The total tail resulting from the three main alpha peaks can be represented by

$$N_i = C_1 e^{-S(x_{p1}-x_i)} + C_2 e^{-S(x_{p2}-x_i)} + C_3 e^{-S(x_{p3}-x_i)} \qquad (20)$$

with

N_i = counts in the total tail in channel i

S = slope of tail as was defined by De Regge

x_{p1}, x_{p2}, x_{p3} = channel number of peak 1, peak 2, peak 3, respectively

C_1, C_2, C_3 = relative abundance of peak 1, peak 2, peak 3, respectively

x_i = channel number of interest

Peak 1 = 5.486 MeV peak of Am^{241}

Peak 2 = 5.443 MeV peak of Am^{241}

Peak 3 = 5.389 MeV peak of Am^{241}

The slope S was calculated by using a least squares fit on the tail of the Am^{241} spectrum. The peak locations were known and the constants C_1 and C_2 could be written in terms of C_3. The constant C_3 could be calculated after substituting a known value for N_i, along with the corresponding channel number, into Eq(20). With C_3 known, the tail resulting only from the 5.486 MeV peak could be calculated. The point k was visually obtained by extending the line formed by this tail until it intersected line (d-e).

Having obtained the slopes S and R and the value of the point k, the next step was to determine the value of the integration constant K in Eq(15). The value of K was calculated by substituting a few values of C(i) in Eq(15) with the real content of a few undisturbed channels near the top of the 5.486 MeV peak. The mean value of K was substituted back into Eq(15) to determine the intermediate channel contents between the tail and the top of the peak.

The values resulting from Eq(15) were checked against one important criterion. Since the actual data was being used to determine a reference peak shape, it would be necessary to require that the contents in every channel calculated by Eq(15) be less than or equal to the contents in the corresponding channel of the real spectrum. If the calculated peak violated this criterion, the peak would be considered invalid. Several different Am^{241} alpha spectra were analyzed using a reference peak obtained from Eq(15). The results of one such analysis are listed in Table I. The results from this analysis are not

directly comparable to those obtained by De Regge because his results represent an average of 13 separate measurements. Only a few of the many analyzes performed using the simplified method were able to satisfy the above criterion and so this method was not used.

Table I

Am^{241} Analyzed Using Reference Peak Obtained by Eq(15) and Simplified De Regge Method

	Alpha I	Alpha II	Alpha III
Peak energy	5.486 MeV	5.443 MeV	5.389 MeV
Peak area	240799	37749	5187
Branching factor *	86.0%	12.7%	1.3%
Computed branching factor	84.4%	13.2%	1.8%
De Regge's computed branching factor	81.8%	14.5%	3.7%

*(From Ref 4:435)

Test Series III

This series of tests involved using the ability of Program ALPHAFIT to accept as reference peak as a table of values specifying the peak shape channel by channel. The tests series evolved around the single alpha emitter, Po^{210}. There were several desired objectives in using Po^{210}. These objectives included reproducing De Regge's work, with hopes of obtaining new constants, which would allow more reliable reproduction of the reference peak in different spectra and evaluating the change

of the resulting peak shape with source thickness. However, before any of these steps were begun, a series of tests were performed in which an actual Po^{210} spectrum was used as a reference peak. The empirical expression, developed by De Regge, was an approximation to a single alpha peak such as obtained from Po^{210}. The best fit that could be obtained would result when the mathematical expression exactly described the single alpha peak. De Regge states that alpha peaks have the same shape independent of their energy when thin sources are used (Ref 2:271). If this assumption is viable, then the limit of precision of the procedure developed by De Regge can be quickly determined by using the single alpha peak (such as obtained from Po^{210}) as the reference peak in the analysis. The results of this analysis are listed in Table II. Using Po^{210} directly as a reference peak did not seem to give better results than those obtained by De Regge's method. The larger error in branching ratios could have resulted from the effects of varying source thicknesses. The resulting error could mean that the sources are of different thicknesses and do not qualify as a thin source; hence, the sources are not expected to be fit using Po^{210}. The variations in source thicknesses are clearly evident in the analysis of Po^{210} - 2 using Po^{210} - 1 as a reference peak. The residual is very large and is due to a different source thickness and a different level of source contamination. A much improved analysis is expected to result when the sources are nearly the same thickness.

Table II

Isotopes Analyzed Using Po^{210} - 1 Directly

as the Reference Peak

Po^{210} - 1	Alpha I		
Energy (MeV)	5.305		
Computed Peak Area =	302894		
Actual Peak Area =	302946		
Residual =	52	RPE_A =	0.02%
$3\sqrt{A}$ =	1651	$RPE_{\sqrt{A}}$ =	0.55%

Am^{241}	Alpha I	Alpha II	Alpha III
Energy (MeV)	5.486	5.443	5.389
Computed Peak Area	811711	80328	1178
Branching Factor	86%	12.7%	1.3%
Computed Branching Factor	90.9%	8.9%	0.13%
Computed Total Area =	893217		
Actual Total Area =	898127		
Residual =	-4910	RPE_A =	0.55%
$3\sqrt{A}$ =	2843	$RPE_{\sqrt{A}}$ =	0.32%

Pu^{240} - 1	Alpha I	Alpha II	Alpha III	Alpha IV
Energy (MeV)	5.499	5.456	5.168	5.123
Computed Peak Area	21939	8928	702697	493291
Branching Factor	0.1224%	0.0476%	74.75%	23.6%
Computed Branching Factor	1.8%	0.73%	57.3%	40.2%

Table II (cont.)

Pu^{240} - 1 (cont.)			
Computed Total Area	= 1229505		
Actual Total Area	= 1226633		
Residual	= 2872	RPE_A	= 0.23%
$3\sqrt{A}$	= 3323	$RPE_{\sqrt{A}}$	= 0.27%

Pu^{240} - 2	Alpha I	Alpha II	Alpha III	Alpha IV
Energy (MeV)	5.499	5.456	5.168	5.123
Computed Peak Area	2501	514	90664	30760
Branching Factor	0.1224%	0.0476%	74.75%	23.6%
Computed Branching Factor	2%	0.41%	72.9%	24.7%

Computed Total Area	= 127271		
Actual Total Area	= 125341		
Residual	= 1930	RPE_A	= 1.54%
$3\sqrt{A}$	= 1062	$RPE_{\sqrt{A}}$	= 0.85%

Po^{210} - 2	Alpha I		
Energy (MeV)	5.305		
Computed Peak Area	= 8745688		
Actual Peak Area	= 8761782		
Residual	= -16094	RPE_A	= 0.18%
$3\sqrt{A}$	= 8880	$RPE_{\sqrt{A}}$	= 0.10%

Table II (cont.)

Composite Spectrum (Po^{210} - 2, Am^{241}, Pu^{240} - 2)

Am^{241}	Alpha I	Alpha II	Alpha III	
Energy (MeV)	5.486	5.433	5.389	
Computed Peak Area	853899	80306	946	
Branching Factor	86%	12.7%	1.3%	
Computed Branching Factor	91.3%	8.6%	0.1%	
Computed Total Area	= 935151			
Actual Total Area	= 898127			
Residual	= 37024		RPE_A = 4.12%	
$3\sqrt{A}$	= 2843		$RPE_{\sqrt{A}}$ = 0.32%	

Composite Spectrum (cont.)

Pu^{240} - 2	Alpha I	Alpha II	Alpha III	Alpha IV
Energy (MeV)	5.499	5.456	5.168	5.123
Computed Peak Area	0	0	60259	15170
Branching Factor	0.1224%	0.0476%	74.75%	23.6%
Computed Branching Factor	0%	0%	79.9%	20.1%
Computed Total Area	= 75429			
Actual Total Area	= 125341			
Residual	= -49912		RPE_A = 39.82%	
$3\sqrt{A}$	= 1062		$RPE_{\sqrt{A}}$ = 0.85%	

Table II (cont.)

Composite Spectrum (cont.)		
Po^{210} - 2	Alpha I	
Energy (MeV)	5.305	
Computed Peak Area	= 1499604	
Actual Peak Area	= 1810354	
Residual	= -310750	RPE_A = 17.17%
$3\sqrt{A}$	= 4036	$RPE_{\sqrt{A}}$ = 1.30%

The last set of tests in Test Series III involved using an entire spectrum of an isotope as a reference peak. The composite spectrum to be analyzed is known to contain certain isotopes (Pu^{240} - 2, Po^{210} - 2, Am^{241}). Several experiments were performed in which the spectrum from each isotope was obtained. The three spectra were then added together to simulate a composite spectrum containing the three isotopes. During the analysis, the spectrum from each isotope was used as the reference peak for that isotope. The results of this analysis are listed in Table III.

Table III

Composite Spectrum Analyzed Using Respective Spectrum from each Isotope as the Reference Peak

Composite Spectrum (Po^{210} - 2, Am^{241}, Pu^{240} - 2)

	Computed Area	Actual Area	Residual	$3\sqrt{A}$
Am^{241}	2712695	898127	1814568	2843
Pu^{240} - 2	2578378	125341	2453037	1062
Po^{210} - 2	1995679	1810354	185325	4036

The residuals resulting from this analysis are well above the desired limit. This error is suspected to have resulted from not utilizing the program's full capability. The analysis was performed as follows:

a) Spectrum to be analyzed read into program

b) Reference peak (entire spectrum of one isotope) read into program

c) Reference peak fit to the data and results printed out

d) Program cleared

e) Spectrum to be analyzed read back into program

f) Next reference peak read into program

g) Reference peak fit to the data and results printed out

h) etc.

A better analysis would result if after the spectrum to be analyzed has been read into the program all three reference peaks were read into the program simultaneously. The program, working up to its full potential, could then vary the relative positions and amplitudes of the reference peaks to obtain the best fit possible.

V. Conclusions and Recommendations

Throughout this thesis, reference was made to the "proper reference peak". The "proper reference peak" is one which best represents the parent population. The "proper reference peak" was used in Test Series I. The spectra in these tests were the parent populations, statistically varied to simulate actual experimental spectra. However, this was done with the qualification that both the reference peak and the spectra were from the same type of source, having the same thickness and backing material.

The ability of Program ALPHAFIT to fit unknown alpha spectra depends upon the ability of the user to find the "proper reference peak". In order to find the "proper reference peak", one needs to study a single undisturbed alpha peak. This was done in the past using Po^{210} (Ref 2:269-280). Even after using the single alpha peak, De Regge had to try to find some empirical function which would allow him to approximate part of the peak. This approach gives good results, but errors result due to the assumptions made by De Regge. Most of the error arose from the empirical function used to represent the peak. Some error could have arisen from the assumption that a complex alpha spectrum is composed of individual alpha peaks which do not interfere with each other, but only add linearly to one another. With the aid of Program ALPHAFIT, the approximations used in trying to find an analytical function to describe the alpha peak are circumvented. Instead, the single alpha peak

from Po^{210} can be directly used by the program to analyze complex alpha spectrum. However, the assumption that complex spectra can be linearly composed of single alpha peaks must still be used. If this is true and if it can be assumed for the moment that for sufficiently thin sources (Ref 2:269-280) the alpha peaks will look the same, then ALPHAFIT should give the most precise results obtainable assuming the Po^{210} alpha peak is obtained by the same detector.

The last series of tests performed were based on the use of an entire spectrum as a reference peak. This would allow circumvention of both approximations made by De Regge. No empirical function would be needed, nor would there be a need for the assumption of linear addition of single alpha peaks. This should allow the most precise analysis possible. The fact that large errors resulted in the first attempt to apply this method should not hinder its further development. Perhaps a spectrum stripping approach would be advisable in this case.

The application of either method requires known samples of high activity to obtain good statistics in the tail region. If the same isotope is to be used to obtain this high activity source, it will require either more area or a thicker source. This is expected to reduce the effectiveness of the reference peak, because the peak shape will change. The change in peak shape should be relatively unchanged if thin sources are used (Ref 3:2043-2047). The exact error incurred would require further tests using varying source thicknesses.

At this time, there appear to be three different methods

which would allow a possible solution to the alpha fitting problem:

I. Reproduce De Regge's work to determine the change in peak shape with source thickness.

II. Investigate further the possibility of using a single alpha emitter such as Po^{210} as a reference peak.

III. Investigate further the possibility of using each respective spectrum in the composite spectrum as a reference peak.

It would be advantageous to include a correction factor for source thickness in each of these methods. This could be accomplished with a library of reference peaks for sources of various thicknesses. An example of such a library could be taken from data such as is found in Figure 2. Knowing a few parameters, such as the shape of the high energy edge of the peak or the full width at half maximum, would allow the user to enter the library and pick the appropriate reference peak. If a sufficient number of reference peaks are catalogued, linear interpolation could be assumed between reference peaks. This would provide an unlimited number of possible reference peaks for a variety of source thicknesses.

Bibliography

1. Bevington, Phillip R. Data Reduction and Error Analysis for the Physical Sciences. New York: McGraw-Hill Book Co., 1969.

2. De Regge, P. "Analysis and Interpretation of Gamma and Alpha Spectra with a Small Real-Time Computer." Nuclear Instruments and Methods, 102:269-280 (February 1972).

3. Kirby, H. W. "Residue Absorption-V Separation of RaD(^{210}Pb) from RaE(^{210}Bi) and RaF(^{210}Po)." J. Inorg. Nucl. Chem. 35:2043-2047 (July 1972).

4. Lederer, C. M., J. M. Hollander, and I. Perlman. Table of Isotopes (Sixth Edition). New York: John Wiley & Sons, Inc., 1967.

5. Price, William J. Nuclear Radiation Detection (Second Edition). New York: McGraw-Hill Book Co., 1964.

6. Watt, D. E., and D. Ramsden. High Sensitivity Counting Techniques. New York: Macmillian Company, 1964.

7. W. C. Davidon, Argonne National Laboratory Report ANL-5990 (Rev. 2), 1966 (unpublished).

APPENDIX A

Program ALPHAFIT

Main Program. The main program controls the reading of the input cards, initializes variables, checks for error conditions, and prepares the data for analysis.

All of the data is read in the main program except for the spectrum data set, which is obtained from Subroutine SPCTRM. A subroutine, named ARYODR, is called to rearrange background points and peak positions into ascending order of abscissas.

As the data is prepared for analysis, the main program establishes the logic for selecting a reference peak, estimating peak positions, and removing background. Two subroutines, named BGRND and REFPEK, are called for establishing the background and the reference peak shape, respectively. Afterwards, a new spectrum with background subtracted is computed with the requirement that none of the computed ordinates be less than zero.

Before analysis of the peaks begins, a final check is made to determine whether the estimated peak locations are in the range of the spectrum. Peaks outside the range are deleted from further processing.

Subroutine RESLTS. Subroutine RESLTS is then called to process the data. Subroutine RESLTS transmits the spectrum to a subroutine, called PREPAR, which establishes the initial error matrix, the weights for the data points, and the convergence

criterion. On returning from Subroutine PREPAR, the normalized fitted peaks are summed to obtain the areas. A printout of the channel number, the raw data, the background, the normalized individual peaks (with background included), and the composite spectrum of the fitted peaks can be obtained by the user upon request.

A final summary page lists the information characterizing the spectrum and tabulates:

a) peak position (channel number),

b) error in peak position (channels),

c) number of counts in the peak,

d) statistical error in the number of counts computed by the program during analysis procedures,

e) sum of the background underneath the peak, and

f) estimated error in the number of counts (this is the square root of the sum of the counts and the background).

Subroutine REFPEK. The one characteristic that made this program look promising was the ability to input any peak shape. This reference peak is not obtained from an analytical function but is expressed as a table of values specifying the peak shape, channel by channel, with linear interpolation assumed between channels.

The reference peak is read into the computer in the main program, and then evaluated by Subroutine REFPEK. This subroutine uses parameters, such as peak width and shape, to

characterize the reference peak. The parameters used are the total width in channels and the distances DELTA1 and DELTA2 shown schematically in Figure 3.

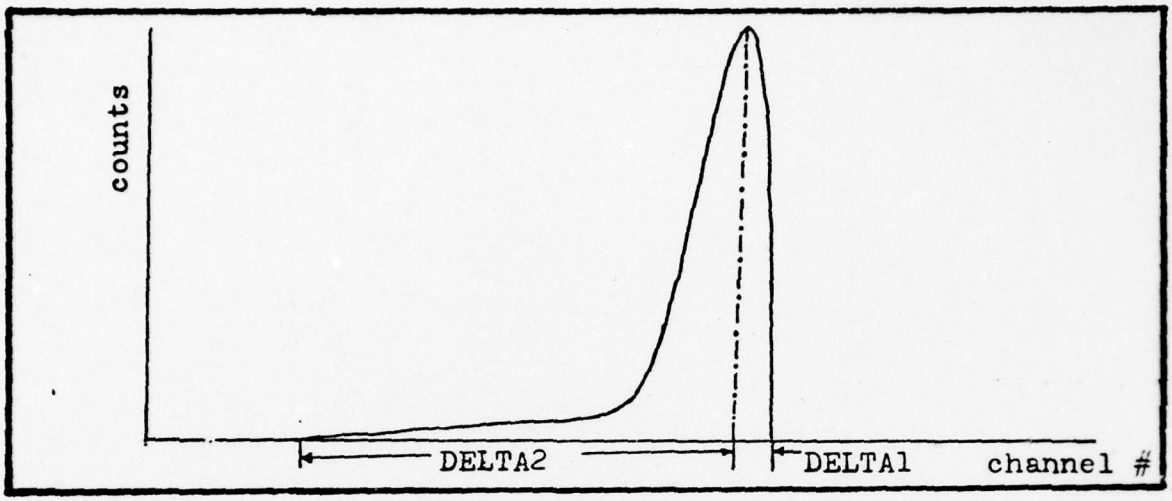

Figure 3. Reference Peak Shape

Subroutine BGRND. Three options are available for removing backgrounds from the spectrum. One option is completely automatic; the other two require information from the user.

Background option I allows the user to specify coordinates of a set of background points throughout the spectrum. Subroutine BGRND then calculates a continuous line that passes through all of these points. The regions between the points are calculated using Lagrange's three-point interpolation formula. Three successive points are used to calculate a curve between the first two points. The first point is then dropped, and the next three successive points are used to calculate the next section. This results in a final curve which is a patchwork of parabolas. The computed background line is continuous,

but its derivative may be discontinuous at each background point. The background is never allowed to be less than zero.

With background option II, the spectrum can be divided into sections with a constant background value in each section. The limits of the sections and the background value of those sections are supplied by the user. This option is useful when the user desires to have a constant background for the entire spectrum.

Background option III, the automatic background option, requires that the estimated locations of the peaks be supplied. Subroutine BGRND examines the regions between such peaks and excludes the channels that contain the tails of the peaks. If such a region is longer than ten channels, it is divided into subregions of about ten channels each. The abscissa of a background point is taken to be the midpoint of the abscissas of the subregion, and the ordinate of a background point is taken to be the average of the ordinates of the data points in the subregion. Since most physical spectra have backgrounds that decrease as the channel number increases, a constraint is imposed on the background points. The ordinate of each new background point $Y_{b,i}$ is compared with the ordinate of the last background point $Y_{b,i-1}$. If the new background point exceeds the value $Y_{b,i-1} + 2\sqrt{Y_{b,i-1}}$, the point is rejected. After at most fifty background points have been selected, a subroutine, named LSQPOL, applies the method of least squares to compute a polynomial of order less than four through the background points.

APPENDIX B

INPUT CARDS FOR PROGRAM ALPHAFIT

Column	Variable		Value	Usage
CARD 1.	Title Card			
	TITLE (1), I = 1, 8			
	FORMAT (8A10)			
1-80	TITLE	=	Any alphanumeric string.	
NOTE:	If columns 1-4 are blank, the program terminates. The program also terminates on an end-of-file card.			
CARD 2a.	Option Control Card			
	NBACK, NPKRD, NREF, NSSW1, NSSW2, MAXREF			
	FORMAT (I4, 4I2, I4)			
1-4	NBACK	=	0	Background determined automatically by program.
		=	+n	Background option I. The X and Y coordinates for n background points will be read in; program calculates a curve passing through all points.
		=	-n	Background option II. n background intervals will be read in (background is a constant between the limits of each interval).
NOTE 1:	$n \leq 50$.			If $n > 50$, the program will truncate it to 50.
NOTE 2:	$n \geq 3$ for background option I (positive sign). But also see Note 2 for card 3.			
5-6	NPKRD	$\geq$	+1	Initial peak positions to be read, as values of channel number.

7-8	NREF	=	0	Reference peak to be selected from spectrum. (This option is generally not recommended.)
		=	-1	Reference peak values to be read from separate cards.
10	NSSW1	=	0	Suppress printed output from variable-metric-minimization routines. (Standard!)
		=	1	Print the v.m.m. calculations.
12	NSSW2	=	0	Suppress printed output of raw data, resolved peaks, and composite spectra.
		=	1	Print the above.
13-16	MAXREF	=		The maximum number of channels in the reference peak.

CARD 2b. Option Control Card

KEPREF, KEPDAT

FORMAT (I1, 3x, I1)

1	KEPREF	=	0	New reference peak used for each spectrum analyzed.
		=	1	Allows the reference peak to be kept for next analysis.
5	KEPDAT	=	0	New data spectrum to be analyzed.
		=	1	Allows the data spectrum to be kept for next analysis.

CARD 3. Background Data Cards (Not used for NBACK = 0.)

DB(I), BACK(I), I = 1, NBACK

FORMAT (16F5.0)

1-5	DB(I)	=	For NBACK > 0 (option I):

11-15, etc.			DB(I) is the channel number at which a background value is to be specified. For NBACK < 0 (option II): DB(I) is the channel number at the lower end of the Ith interval for which a background value is to be specified. DB(1) is supplied by the program and may be left blank.
6-10	BACK(I)	=	The value of the background for the Ith background position (NBACK > 0), or for the Ith background interval (NBACK <0).

NOTE 1: The pairs DB(I), BACK(I) may be given in any order. The program will rearrange them in increasing order of DB(I).

NOTE 2: For NBACK > 0, the program requires backgrounds for the first and last channels of data. If not given explicitly, the program will use BACK (1) for the first channel, and BACK (NBACK) for the last channel. These program-supplied values may be counted for meeting the minimum requirement of 3 background points.

CARD 4a. Reference Peak Values Card (Use only for NREF < -1.)

N

FORMAT (I4)

1	N	=	The number of channels in the reference peak.

DUMCHN, (STOREF(J+K), K = 1, 10)

FORMAT (F6.0/10(F6.0, 2x))

1-6	DUMCHN	=	Every tenth channel number of the reference peak. These values are not needed in the reference peak and so are not stored. This allows cards punched from MCA to be read without conversion.

1-6 9-14 etc.	STOREF(J+K)	=	The number of counts in the (J+K)th channel of the reference peak, reading from the back edge to the front edge.

CARD 4b. Reference Peak Parameter Card (Use only if NREF = 0.)

STOIPR, DELTA1, DELTA2, DELTA3

FORMAT (4F10.5)

1-10	STOIPR	=	The channel number of the maximum count in the reference peak.
11-20	DELTA1	=	Channels from the front (high-energy) edge of the reference peak to the "third-height" position on the front edge.
21-30	DELTA2	=	Channels from the back (low-energy) edge of the reference peak to the third-height position.
31-40	DELTA3	=	Channels from STOIPR to the third-height position.

NOTE: For MCA operation, the "third-height" position is defined as STOIPR and hence the program sets DELTA3=0.0.

CARD 5. Standard Spectrum Data Set

D1, (Y(I), I = 1, 10)

FORMAT (F6.0/10(F6.0, 2x))

1-6	D1, D	=	Every tenth channel of the spectrum.
1-6 9-14 etc.	Y(I)	=	The number of counts in the Ith channel of the spectrum.

CARD 6. Peak Position Cards (Use with NPKRD > +1.)

PEKPOS(I), IFIXPK(I)

FORMAT (F9.4, I1)

1-9	PEKPOS(I)	=	The estimated third-height location of the Ith peak to be considered by the program, specified in channel number.
10	IFIXPK(I)	= 0 or blank	The program will adjust PEKPOS(I) for the best fit to the data. (Standard option.)
		> 1	PEKPOS(I) will be held fixed by the program.

NOTE: The cards may be in any order. The program will rearrange them into ascending order of PEKPOS(I).

CARD 7. Peak Position Termination Card

PEKPOS(I) < -1.0 This will terminate peak locations and the program will process a new set of data, beginning with Card 1.

APPENDIX C

RECOMMENDATIONS FOR INPUT

The following suggestions are intended to aid the user in setting up the input card decks to ALPHAFIT.

Backgrounds

The automatic background option is sometimes capable of providing a reasonable estimate of the background, but it can also produce very unrealistic results. The use of the automatic option is not recommended if high-quality results are desired. Background option I (NBACK > 0) gives the user the maximum control over the background curve. If enough points are specified, the background can be tailored to any specification.

With background option II (NBACK = -1) constant backgrounds can be entered into the program. Option I can also be used with NBACK = +1 if DB(1) specifies any abscissa in the middle of the spectrum and BACK(1) specifies the background value.

Peak Selection

The option that requests the program to hold positions of peaks fixed while obtaining their areas is not generally recommended. It is useful if the program has troubles in separating closely-spaced peaks whose positions are known in advance. However, the positions of peaks are almost never known a priori. Even if their energy values are precisely known, experimental uncertainties and insufficient yields may make their positions in a spectrum poorly known.

Printout Options

The input NSWW1 = 1 produces messages from the variable-metric-minimization package. This is useful for error tracing or debugging. Otherwise, set NSSW1 = 0.

The input NSSW2 = 1 produces a printout of the channel numbers, raw data, and individual peaks fit to the raw data. It is sometimes useful if the user wishes to make minor corrections to the final results from ALPHAFIT by manually summing the counts in a peak.

APPENDIX D

INTERPRETING THE OUTPUT

Special Messages

Most of the printed output is self-explanatory. In addition to the error messages indicating improper data (listed in the descriptions of the utility subroutines), a few other messages can be produced under special conditions.

nn Peaks Deleted. Some of the peak positions that were read in are not in the range of abscissa values.

Epsilon Too Small--Cannot Converge For Peaks At xxx, yyy. Twenty-five complete iterations have been made by the variable-metric package in an attempt to minimize the function F for the peaks located at the positions listed. Convergence was not achieved and the results of the last iteration are returned to the calling programs. Normally, these are sufficiently accurate. However, this message is sometimes produced if the spectrum is very complex and either too many or too few peaks are specified. One should revise the estimates of the peak positions and rerun the program.

Results of the Peak-Fitting Analysis

The final printed summary of results should be examined for signs that the calculated fits to the data may not be reliable. If necessary, the input deck can be revised and another pass made.

Errors. One can roughly estimate the errors expected for

the final positions and areas of the peaks and compare these with the calculated errors. Large discrepancies require attention. The expected error in the area (NUMB. COUNTS) A is $\sqrt{A}$. The expected error in the peak position is roughly FWHM/(2.5$\sqrt{A}$), where FWHM is the full-width at half maximum of the peak.

Normally, the positions and areas of the peaks will be determined much more precisely than the listed errors would indicate. A large discrepancy between estimated and listed error is thus only a sign that the program experienced difficulties in the analysis, not that the answers are necessarily unreliable.

Negative Peaks. The program sometimes produces peaks with negative areas. This is usually a sign that ALPHAFIT has been asked to place too many peaks in a small region. Some should be eliminated and the data should be reanalyzed. If the user intends to have all the peaks he requested, a revised set of estimated peak positions can sometimes eliminate negative peaks.

Peaks with Zero Areas and Errors. The printout may show that some peaks have areas and errors which are exactly zero. This results from a spurious condition. During the variable-metric analysis, these peaks have been moved outside the range of the spectrum in the work area (not outside the total spectrum) and therefore have zero amplitudes. The errors are arbitrarily set to zero. The cause is usually the same as for negative peaks and should be treated accordingly.

Appendix E:

Program ALPHAFIT Listing

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```
      PROGRAM ALPHET(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,PUNCH,
     1  TAPE7=PUNCH,TAPE3)
      PROGRAM ALPHAFIT WAS OBTAINED FROM PROGRAM AUTOFIT WRITTEN BY
      J.P. COMFORT OF ARGONNE NATIONAL LABORATORY
      THIS PROGRAM ALLOWS THE FOLLOWING:
      A MAXIMUM OF 2100 CHANNELS FOR A REFERENCE PEAK
      A MAXIMUM OF 2100 CHANNELS FOR A SPECTRUM
      A MAXIMUM OF 50 CHANNELS FOR A BACKGROUND  INPUT
      COMMON /A00/ W11(732),NSSW1,NSSW2
      COMMON /A02/ DUMMY(161), STORV1(2100), RAWX(2100), ITIMES, NNX
      COMMON/A03/ TITLE(20),PEKPOS(20),IFIXPK(20),BETA,GSTATE,
     1  GSIGVAL, MT, NCALC, IGS, L0
      COMMON /A04/ INTREF(20,10),STOREF(2100),DELTA1,DELTA2,DELTA3,
     1  BIGIPR, REFMAX, IO1, IO2, IOT, NB, NF, NREF
      COMMON /A05/ BACK2(2100), BB(50), BACK(50), NJ, NBACK, NPKRD
      COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, OFTEN,
     1  NOFTEN, NCHANN, II, IJ, ISPECT, IFMT, IERR,MAXREF,MAXP2
      COMMON /OPTN/ KEPREF,KEPDAT
      DIMENSION PEESTO(2100)
      EQUIVALENCE (IBLNK,BLNK,DBLNK)
      DATA(DBLNK=8H          )
         ...START CALCOMP AND GET DATE...
      IERR = 0
       CALL DATE(TODAY)
      GO TO 50
         ...TERMINATE PROGRAM...
   45 WRITE(6,101)
  101 FORMAT(3X,18H  ENDPLOT EXECUTED)
      STOP
         ...READ AND WRITE TITLE CARD.  EXIT ON E.O.F...
   50 READ(5,10)          (TITLE(I),I=1,8)
       IF(EOF(5)) 45,+9
   49 IF (TITLE(1).EQ.BLNK) GO TO 45
      WRITE(6,30) (TITLE(I),I=1,8 ),TODAY
         ...INPUT OF DATA...
      READ(5,12)        NBACK,NPKRD,NREF,        NSSW1,NSSW2,MAXREF
      KEPREF IS AN OPTION TO ALLOW THE USER TO KEEP THE SAME REFERENCE
      PEAK FOR ALL ANALYSIS
      KEPREF.GT.0 ALLOWS THE USE OF THE SAME REFERENCE PEAK FOR ENTIRE
      ANALYSIS
      KEPREF.EQ.0 REQUIRES A NEW REFERENCE PEAK WITH EACH SPECTRUM
      ANALYZED
      KEPDAT IS AN OPTION TO ALLOW THE SAME DATA SET TO BE USED FOR ALL
      ANALYSIS.
      KEPDAT .GT.0 ALLOWS THE SAME DATA SET TO BE USED FOR THE ANALYSIS.
      KEPDAT .EQ.0 REQUIRES A NEW DATA SET FOR EACH ANALYSIS.
      READ*,KEPREF,KEPDAT
      MAXP2 = MAXREF + 2
      IF (NREF.GT.10) NREF = 10
      WRITE(6,32)        NBACK,NPKRD,NREF,        NSSW1,NSSW2,MAXREF
      PRINT*," KEPREF = ",KEPREF,"          KEPDAT = ",KEPDAT
```

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```
      IF (NBACK) 71,110,80
   70 NJ = -NBACK
      NBACK = 2
      GO TO 90
   80 NJ = NBACK
      NBACK = 1
   90 IF (NJ.GT.50) NJ = 50
      READ(5,14) (DB(I),BACK(I),I=1,NJ)
      IF (NJ.GT.1) CALL ARYORD(DB,BACK,NJ,2)
         ...INITIALIZATION...
  100 LO = 0
      STOIPR = 0.0
      DO 105 I=1,20
  105 IETYPK(I) = 0
      DO 110 I=1,MAXREF
  110 STOREF(I) = 0.0
         ...MORE DATA INPUT...
      IF (MREF) 120,130,150
  120 IF(KEPREF.GT.0)GO TO 778
      READ*,N
      IF(N.GT.MAXREF) N = MAXREF
      DO 777 I=1,N,10
      J = I-1
      READ 111,DUMCHN,(STOREF(J+K),K=1,10)
  111 FORMAT(F6.0/10(F6.0,2X))
  777 CONTINUE
      NSTOR = N
      DO 77 I =1,N
      REFSTO(I) = STOREF(I)
   77 CONTINUE
      GO TO 1000
  778 DO 99 I = 1,NSTOR
      STOREF(I) = REFSTO(I)
   99 CONTINUE
 1000 CONTINUE
      GO TO 150
  130 READ(5,18) STOIPR,DELTA1,DELTA2,DELTA3
  150 CONTINUE
         ...GET A STANDARD SPECTRUM DATA SET...
      IF(KEPDAT.GT.0) GO TO 175
  170 CALL SPCTRM
  175 IF (IERR.GT.0) GO TO 45
      WRITE(6,34) NCHANN
      DELTA3 = 0.0
         ...READ PEAK POSITIONS, DISTANCE
  200 DO 220 I=1,21
  210 READ(5,24) PEKPOS(I),IETYPK(I)
      IF (PEKPOS(I).LE.-1.) GO TO 230
  220 CONTINUE
      NT = 20
      GO TO 240
```

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```
      NT = T - 1
      IF (NT.GT.1) CALL ARYCOR(PEKPOS,IFIXPK,NT,2)
      DO 351 I=1,NCHANN
  351 RAWX(I) = COUNTS(I)
          ...CALC. BACKGROUND, SELECT REFERENCE PEAK AND PICK PEAKS...
      NNX = 0
      IF ((NBACK.EQ.0).AND.(NPKRD.EQ.0)) GO TO 440
      IF (NBACK.EQ.0) GO TO 370
      IF (DB(1).LT.DIST(1)) DB(1) = DIST(1)
      IF (DB(NJ).GT.DIST(NCHANN)) DB(NJ) = DIST(NCHANN)
  370 CALL BGRND
      NNX = NNX + 1
      DO 420 I=1,NCHANN
      IF (RAWX(I)) 420,420,410
  410 RAWX(I)=RAWX(I)-BACK2(I)
      IF(RAWX(I).LT.0.0) RAWX(I) = 0.0
  420 CONTINUE
  440 CALL REFPEK
      IF (NPKRD.NE.0) GO TO 500
  460 DO 470 I=1,NT
  470 PEKPOS(I) = PEKPOS(I) + DELTA3
      IF (NNX) 370,370,520
  500 WRITE(6,38)
      GO TO 530
  520 WRITE(6,42)
      ... MAKE SURE THAT ALL PEAKS ARE IN THE RANGE OF THE SPECTRUM
  530 M = 0
      DO 550 I=1,NT
      IF ((PEKPOS(I)-DELTA2-2.*OFTEN).LT.DIST(1)) GO TO 550
      IF ((PEKPOS(I)+DELTA1+2.*OFTEN).GT.DIST(NCHANN)) GO TO 550
      M = M + 1
      PEKPOS(M) = PEKPOS(I)
      IFIXPK(M) = IFIXPK(I)
  550 CONTINUE
      IF (M.GE.NT) GO TO 580
      I = NT - M
      WRITE(6,44) I
  580 NT = M
      WRITE(6,42) (PEKPOS(I),I=1,NT)
      DO 600 I=1,NCHANN
  600 STORV1(I) = BACK2(I)
      CALL RES_TS
      GO TO 50
   1  FORMAT(8A10)
   12 FORMAT(   I4,4I2,I4          )
   14 FORMAT(15F5.0)
   15 FORMAT(I3,15F5.0)
   18 FORMAT(4F10.5)
   24 FORMAT(F9.4,I1,F10.5)
   30 FORMAT(1H1,1X,8A10,10X,A10)
   32 FORMAT(10H                4X8HNPBCK = I4,4X8HNPKRD = I2,4X7HNREF = I2
     1,4X7H            4X8HNSSW1 = I2,4X8HNSSW2 = I2,4X8H1AXREF = I4)
```

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```
 3, FORMAT(11H0 NCHANN = I3,5X7H                    )
 33 FORMAT(35H0 INITIAL GUESSES OF PEAK POSITIONS)
 41 FORMAT(40H0 CALCULATED ESTIMATES OF PEAK POSITIONS)
 42 FORMAT(11F12.7)
 44 FORMAT(1H0,I4,14H PEAKS DELETED)
    END
    SUBROUTINE RESLTS
    DIMENSION FMT(3), WORD(21)
    DIMENSION PEKPOS(200), PKBACK(200), XSECTS(200), XSECPO(200),
   1 DELT(200), EX(200)
    COMMON /A00/ V11(552), IHOLD(20), NSSW1, NSSW2
    COMMON/A01/STORST(2102,20),S(2102),IZSTRT(20),IZSTOP(20),DUM(3538)
    COMMON /A02/ SIGMA(20), PERR(20), PEKSTO(21), STORHH(20),
   1  XINTIS(20), INDEX(20), INITAL(20), IFINAL(20), STORV1(2100),
   2  RAWX(2100), ITIMES, NNX
    COMMON/A03/ TITLE(20),PEKPOS(21),IFIXPK(20),BETA,GSTATE,
   1  GSDVAL, NT, NCALC, IGS, LO
    COMMON /A04/ INTREF(20,10),STOREF(2100),DELTA1,DELTA2,DELTA3,
   1  STOIRR, REFMAX, IP1, IP2, IDT, ND, NE, NREF
    COMMON /A05/ BACK2(2100), B2(50), BACK(50), NJ, NBACK, NPKBD
    COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, DFTEN,
   1  NOFTEN, NCHANN, II, IJ, ISPECT, IFMT, IERR,MAXREF,MAXP2
    DATA(FMT=8H(1X,F9.4,, 7HF10.2,, 1H , 5HF10.2, 5H/40X,, 8H 9F10.2))
    DATA (WORD                = 8H       9, 8H  10X, 8, 8H  20X, 7,
   1  8H  30X, 6, 8H  40X, 5, 8H  50X, 4, 8H  60X, 3, 8H  70X, 2,
   2  8H  80X, 1, 8H        9, 8H  10X, 8, 8H  20X, 7, 8H  30X, 6,
   3  8H  40X, 5, 8H  50X, 4, 8H  60X, 3, 8H  70X, 2, 8H  80X, 1,
   4  8H        8, 8H  10X, 8)
    DATA (ISS=1HF),(IBLNK=1H )
      ...INITIALIZATION...
    JO = 0
    JOR = 0
    NNY = 1
    NT2 = 1
    NT = 1
    NT1 = NT
      ...STORE INFORMATION AND GET READY TO CALL PREPAR...
 60 DO 70 I=1,NT
    J = NNY + I - 1
    IHOLD(I) = IFIXPK(J)
 70 PEKSTO(I) = PEKPOS(J)
 90 DELTA1 = DELTA1/DFTEN
    DELTA2 = DELTA2/DFTEN
    CALL PREPAR
    DO 140 I=1,NT
    J = NNX + I - 1
141 IFIXPK(J) = IHOLD(I)
    NNY = NNX + NT
    IF (NSSW2.GT.0) WRITE(6,9042)
9042 FORMAT(10H0 DISTANCE,2X8HRAW DATA,2X10HBACKGROUND,2X9HCOMPOSITE,4X
   116HRESOLVED SPECTRA)
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```
      ... CALCULATE AREAS AND ERRORS FOR THIS GROUP...
      DO 91 I=1,MT
      XINTIS(I) = 0.
      DO 3005 J=1,MAXP2
 3005 XINTIS(I) = XINTIS(I) + STOR7(J,I)
      JO=JO+1
      PEAKPOS  (JO)=PERSTO  (I)
      PEAKERR (JO)=SIGMA(I)
      PKBACK(JO) = 0.0
      XSECTS(JO)=XINTIS(I)
   91 XSECER(JO)= XSECTS(JO)*ERR7(I)
      ...ADD BACKGROUNDS AND PRINT THE RESOLVED AND COMPOSITE SPECTRA
      JPP = 0
      DO 7300 I=1,ITIMES
      MOP = JPP + 1
      JPP=MOP+INDEX(I)-1
      MZZ=INITAL (I)
      MMX=IFINAL(I)
      IF (NSSW2.EQ.0) GO TO 1530
      IF(MZZ-MTT) 2011,2011,2012
 2011 MZZ = MZZ - 1
      DO 2012 L = MTT,MZZ
 2012 WRITE(6,FMT)  DIST(L),COUNTS(L),BACK2(L)
 2011 WRITE(6,9082) (PERSTO  (JP),JP=MOP,JPP)
 9082 FORMAT(40X,8E10.2)
 1530 DO 7010 J=MZZ,MMX
      K1 = 0
      K2 = 0
      M = J - MZZ + 1
      STORV1(J) = BACK2(J)
      DO 1310 JP = MOP,JPP
      J2 = JP
      IF ((M.GE.IZSTRT(JP)).AND.(M.LE.IZSTOP(JP))) GO TO 1320
 1310 K1 = K1 + 1
      IF (NSSW2.EQ.0) GO TO 3010
      WRITE(6,FMT) DIST(J),COUNTS(J),BACK2(J)
      GO TO 3010
 1320 DO 1330 JP = J2,JPP
      IF ((M.LT.IZSTRT(JP)).OR.(M.GT.IZSTOP(JP))) GO TO 1340
      JP = JOP + JP
      PKBACK(JP) = PKBACK(JP) + BACK2(J)
 1325 K2 = K2 + 1
      ITT = M - IZSTRT(JP) + 1
      STORV1(J) = STORV1(J) + STOR7(ITT,JP)
      STOR7(ITT,JP) = STOR7(ITT,JP) + BACK2(J)
 1330 S(K2) = STOR7(ITT,JP)
 1340 FMT(3) = NOBR(K1 + 1)
      IF (NSSW2.EQ.0) GO TO 3010
 3009 WRITE(6,FMT) (DIST(J),COUNTS(J),BACK2(J),STORV1(J),(S(K),K=1,K2))
 3010 CONTINUE
      MTT = MMX + 1
```

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```
3311 CONTINUE
     JJJ = JJJ + NT
  99 IF (NSSN2.EQ.0) GO TO 3401
     DO 3400 I=NTT,NCHANN
3400 WRITE(6,FMT)  XTST(I),COUNTS(I),BACK2(I)
        ...PRINT READINGS...
3401 WRITE(6,85) (TITLE(I),I=1,8 ),TODAY
     WRITE(6,200)
 550 DO 560 I=1,JJ
     IPF = IPLNK
     IF (IPEAK(I).GT.0) IPF = ISF
     AREA = XSECTS(I)+PKBACK(I)
     STYERR = 0.
     IF (AREA.GT.0.) STYERR = SQRT(AREA)
     WRITE(6,212) PEKPOS(I),IPF,PEKERR(I),XSECTS(I),XSECER(I),
    1  PKBACK(I),STYERR
 560 WRITE(7,215) PEKPOS(I),XSECTS(I),PKBACK(I),PEKERR(I),XSECER(I)
 130 WRITE(7,230)
     RETURN
  85  FORMAT(1H1,1X,3A10,10X,A10)
 200 FORMAT(/5X4HPEAK,2FX7H    ,19X5HNUMB.,35X4HEST./4X8HPOSITION,6X7H
    1     ,6X5H       ,FX5HERROR,7X6HCOUNTS,12X5HERROR,13X10HBACKGROUND
    2,6X5HERROR/)
 201 FORMAT(3XF9.3,1XA1,3XF8.4,4XF8.4,4XF6.2,5XF8.2,3(4XF8.2))
 202 FORMAT(F8.4,1X,3F10.4,2F10.2,F8.2,F8.1,3XA6,F5.1)
 221 FORMAT(3XF9.3,1XA1,3XF8.4,15XF6.2,5XF8.2,3(4XF8.2))
 222 FORMAT(F8.4,1XF10.4,10X,2F10.2,F8.2,F8.1,3XA6,F5.1)
 213 FORMAT(3XF9.3,1XA1,2FXF6.2,5XF12.2,3(4XF11.2))
 215 FORMAT(F8.4,21X,2F10.2,F8.2,F8.1,3XA6,F5.1)
 230 FORMAT(2H-1)
     END
     SUBROUTINE SPCTRM
  ....READS THE SPECTRUM CARDS AND SETS THE DISTANCE AND COUNT ARRAYS
     DIMENSION YSAV(10)
     COMMON/DATA/X(2100),Y(2100),RUNID,TODAY,FREQ,DELX,NOFTEN,
    1 N,NT,IJ,ISPECT,IFMT,IERR,MAXREF,MAXP2
     COMMON /OPTN/ KEPREF,KEPFAT
  .......  INITIALIZE COUNTS ARRAY TO ZERO
     DO 100 I=1,2100
 100 Y(I)=0.0
     N=10
     DELX = 1.0
  ....  READ IN THE FIRST TEN VALUES OF SPECTRUM ......
 130  READ(5,6) D1,(Y(I),I=1,10)
  ...  LOAD IN NEXT TEN VALUES OF SPECTRUM INTO YSAV  .....
 135  READ(5,6) D,(YSAV(I),I=1,10)
     IF(EOF(5)) 250,75
  75 CONTINUE
  ...  TEST FOR SPECTRUM TERMINATION CARD  .....
 200 IF(YSAV(1).LE.-1) GO TO 250
  ...  TEST FOR ILLEGAL ORDER OF CHANNELS  ...
```

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```
      IF(D.LT.D1) GO TO 230
C.... COMPUTE THE PROPER ARRAY LOCATION FOR THE LAST READ .....
      M1=(D-D1)/DELX + 1.1
      M2=M1 + 9
      IF(M.LT.M2) M=M2
      IF(N.GT.2100) GO TO 235
C...  STORE DATA LOADED IN YSAV INTO NEXT TEN SLOTS OF Y ....
      DO 220 I=M1,M2
      J=I-M1+1
  220 Y(I)=YSAV(J)
      GO TO 135
C.... ERROR MESSAGES ....
  230 WRITE(6,1)D,D1
      GO TO 245
  235 WRITE(6,2) N
  245 IERR=1
      GO TO 300
C.... SET THE DISTANCE VALUES ....
  250 Y(1)=D1
      DO 260 I=2,N
  260 Y(I)=D1 + FLOAT(I-1)*DELX
  300 RETURN
    3 FORMAT(F5.0,2F7.0,8X,F3.0)
    1 FORMAT(6H0 D = ,F9.3,16H LESS THAN D1 = ,F9.3)
    2 FORMAT(11H0 NOMAIN = ,I5,18H GREATER THAN 2100)
    6 FORMAT(F5.0/10(F6.0,2X))
      END
      SUBROUTINE ARYORD(A,B,N,L)
C        ORDERS THE ARRAY A, AND MAKES SAME ORDERING TO B IF L=2.
      INTEGER B
      DIMENSION A(1),B(1)
      NP = N - 1
      DO 50 I=1,NP
      K = I + 1
      DO 50 J = K,N
      IF (A(I)-A(J)) 50,50,20
   20 IF (L-1) 40,40,30
   30 TSAV = B(I)
      B(I) = B(J)
      B(J) = ISAV
   40 SAVE = A(I)
      A(I) = A(J)
      A(J) = SAVE
   50 CONTINUE
      RETURN
      END
      SUBROUTINE REFPEK
C     DETERMINES THE PARAMETERS OF THE REFERENCE PEAK
      COMMON /A02/ DUMMY(101), STORV1(2100), RAUX(2100), ITIMES, NNX
      COMMON /A03/ SKIP(66),LC
      COMMON /A04/ THREF(20,10),STOREF(2100),DELTA1,DELTA2,DELTA3,
     1  STOIPR, REFMAX, ID1, ID2, IDT, NB, NE, NREF
```

```
      COMMON /ADC/ BACK2(2100), DB(50), BACK(50), NJ, NBACK, NDK30
      COMMON /DATA/ FIRST(2100), COUNTS(2100), RUNID, TODAY, FREQ, OFTEN,
     1  NOFTEN, NCHANN, TI, IJ, ISPECT, IEMT, IEPP,MAXREF,MAXP2
      COMMON /OPTN/ KEPREF,KEPDAT
      IF (LO) 10,30,10
   10 IF (NREF) 300,200,300
   30 IF (NREF) 100,200,80
C  SELECT REFSHAPE FROM INTERNAL DATA
   80 DO 90 I=1,20
   90 STOREF(I) = INTREF(I,NREF)
C  FIND LOWER EDGE OF PEAK
  100 DO 110 I=1,MAXREF
      IF(STOREF(I)) 110,110,120
  110 CONTINUE
  120 IMIN = I
      IF (I.GT.1) IMIN = I - 1
C  FIND UPPER EDGE OF PEAK
      I = MAXREF
  130 IF (STOREF(I)) 140,140,150
  140 I=I-1
      GO TO 130
  150 IMAX = I
      IF(I.LT.MAXREF) IMAX = I+1
C  FIND TOP OF PEAK
      REFMAX=0.0
      DO  170 I=IMIN,IMAX
      IF (REFMAX-STOREF(I)) 160,170,170
  160 REFMAX = STOREF(I)
      ITOP=I
  170 CONTINUE
C  FINDS THIRD HEIGHT
      REFTHD = REFMAX/3.
      DO 180 I=ITOP,IMAX
      IF (STOREF(I)-REFTHD) 190,180,180
  180 CONTINUE
  190 RI=I
      OFFSET = (REFTHD-STOREF(I))/(STOREF(I-1)-STOREF(I))
      RTHPOS=RI-OFFSET
      IF (OFTEN.EQ.1.0) RTHPOS = FLOAT(ITOP)
      DELTA1 = (FLOAT(IMAX)-RTHPOS)*OFTEN
      DELTA2 = (RTHPOS-FLOAT(IMIN))*OFTEN
      DELTA3 = (RTHPOS-FLOAT(ITOP))*OFTEN
      RTHPOS = (RTHPOS-1.0)*OFTEN
      STORE = 0.0
  200 IDT=(DELTA2+DELTA1)/OFTEN + 1.1
      ID1=(DELTA1+DELTA3)/OFTEN +0.1
      ID2=(DELTA2-DELTA3)/OFTEN +.1
      NE = NCHANN - ID1
      N9 = ID2 + 1
      IF (NREF) 230,210,230
C  SELECT REFSHAPE FROM RAW SPECTRUM
```

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```
210 KU = (STOIPR-DIST(1))/DFTEN + 0.1
    IIO = KU - II2
    IMIN = 1
    IMAX = IMIN + IDT - 1
    STORE = DFTEN*FLOAT(IIO) + DIST(1)
    RTHPOS = STOIPR + DELTA3
    DO 220 I2=1,IDT
220 STOREF(I2)=DUMMY(IIO+I2)
230 IF (LO) 240,241,310
241 DO 250 I=IMIN,IMAX
250 STOREF(I-IMIN+1) = STOREF(I)
    IF (NNX) 400,400,300
300 WRITE(6,310) DELTA1, DELTA2, DELTA3
310 FORMAT(11HO DELTA1 = ,F9.0,8X9HDELTA2 = ,F9.0,8X9HDELTA3 = ,F9.0)
    IF(KEPREF.GT.0) GO TO 342
    IF(KEPDAT.GT.0) GO TO 342
    WRITE(6,320)
320 FORMAT(15HO REFERENCE PEAK/11H  CHANNEL #,10X7H COUNTS)
    DO 340 I=1,IDT
    WRITE(6,330) STORE,STOREF(I)
330 FORMAT(1XF9.4,10XF10.2)
340 STORE = STORE + DFTEN
342 CONTINUE
    WRITE(6,350) RTHPOS
350 FORMAT(32H  REFERENCE PEAK THIRD HEIGHT = ,F9.4)
400 RETURN
    END
    SUBROUTINE BGRND
    ...CALCULATES THE BACKGROUNDS...
    COMMON /A02/ DF(12), RHO2(52), W(50), X(10), A(10,10),DUMMY(4099)
    COMMON /A03/ TITLE(20),PEAK(20),BLNK(23),NPEAK,NCALC,IGS,LO
    COMMON /A04/ INTREF(20,10),STOREF(2100),DELTA1,DELTA2,DELTA3,
   1  STOIPR, REFMAX, ID1, ID2, IDT, NB, NE, NREF
    COMMON /A05/ BACK2(2100), DB(50), BACK(50), NJ, NBACK, NPKRD
    COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, DFTEN,
   1  NDFTEN, NCHANU, SKIP(5),MAXREF,MAXF2
    DO = DIST(1)
    IF (NBACK-1) 10,700,900
      ...AUTOMATIC BACKGROUND SELECTION...
 10 NP = NPEAK + 1
    IJ = 0
    NJ = 0
    RHO2(NJ) = 1.E10
    DO 200 JJ=1,NP
    IJ = IJ + 1
    IF(IJ-NP) 20,91,400
 20 LOOPK = (PEAK(IJ)-DELTA3-DO)/DFTEN + 1.1
    IF(IJ-1) 40,40,30
 40 NDEL = LOOPK - ID2 - 1
    M1 = 0
    GO TO 100
```

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```
 60 NDEL = IFIX((PEAK(IJ)-PEAK(IJ-1))/OFTEN + 0.1) - IOT
    MA = LOOPK - IO2 - NDEL - 1
    GO TO 100
 80 LOOPK = (PEAK(IJ-1)-DELT(3-00)/OFTEN + 1.1
    NDEL = NCHANN - LOOPK - IO1
    MA = LOOPK + IO1
100 IF(NDEL-10) 200,120,120
120 JBACK = FLOAT(NDEL)/10.0 + 0.2
    JP = NDEL/JBACK
    SHIFT = FLOAT(JP)/2.
    DO 180 I=1,JBACK
    NJ = NJ + 1
    S = 0.0
    DO 140 IP=1,JP
140 S = S + Y(MA+IP)
    RHO2(NJ) = S/FLOAT(JP)
    BACK(NJ) = RHO2(NJ)
    CHECK = RHO2(NJ-1) + 2.*SQRT(RHO2(NJ-1)+1.)
    IF (RHO2(NJ)-CHECK) 160,160,150
150 NJ = NJ - 1
    GO TO 170
160 DE(NJ) = DIST(MA+1) + OFTEN*SHIFT
    DB(NJ) = DE(NJ)
      ...TEST FOR LIMIT OF 50 POINTS AND TAKE APPROPRIATE ACTION...
170 IF (NJ-48) 180,175,400
175 IF (IJ.GE.NP) GO TO 400
    IJ = NP
    GO TO 80
180 MA = MA + JP
200 CONTINUE
400 IF (NJ-3) 410,420,420
410 M = NJ - 1
    GO TO 430
420 M = 4
430 N = NJ
500 MM = M + 1
    DO 510 I=1,N
510 W(I) = 1.0
    CALL LSQPOL(N,M)
    DO 540 I=1,NCHANN
    BACK2(I) = X(1)
    DO 520 IP=1,M
520 BACK2(I) = BACK2(I) + X(IP+1)*DIST(I)**IP
    IF(BACK2(I)) 530,540,540
530 BACK2(I) = 0.0
540 CONTINUE
    GO TO 800
      ...INTERPOLATE THE BACKGROUND THROUGH THE POINTS READ IN...
700 JD1=0
    JD2=0
    IF(DB(1)-DIST(1)) 710,710,705
```

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```
      JC1=1
      DE(1) = DIST(1)
      RHO2(1)=BACK(1)
  710 IF(DIST(NJ)-DIST(NCHANN)) 715,750,750
  715 JC2=1
      DE(NJ+JC1+1) = DIST(NCHANN)
      RHO2(NJ+JC1+1)=BACK(NJ)
  750 DO 755 I=1,NJ
      DE(I+JC1)=DB(I)
  755 RHO2(I+JC1)=BACK(I)
      N=NJ+JC1+JC2
      IF (N.LT.3) GO TO 900
      J=2
      DO 780 I=1,NCHANN
      DIX = DIST(I)
  770 IF(DIX-DE(J+1)) 780,775,775
  775 J=J+1
      IF (J.GE.N) J= J - 1
  780 DEM1=(DE(J-1)-DE(J))*(DE(J-1)-DE(J+1))
      DEM2=(DE(J)-DE(J-1))*(DE(J)-DE(J+1))
      DEM3=(DE(J+1)-DE(J-1))*(DE(J+1)-DE(J))
      BACK2(I)=(DIX-DE(J))*(DIX-DE(J+1))/DEM1*RHO2(J-1)
     1    + (DIX-DE(J-1))*(DIX-DE(J+1))/DEM2*RHO2(J)
     2    + (DIX-DE(J-1))*(DIX-DE(J))/DEM3*RHO2(J+1)
      IF(BACK2(I).LT.0.0) BACK2(I)=0.0
  790 CONTINUE
      WRITE(6,810) (DE(I),RHO2(I),I=1,N)
  810 FORMAT(25H0POINTS USED BY BACKGROUND/(2F12.3))
      GO TO 1000
         ...CALCULATE THE BACKGROUND INTERVALS...
  900 IJ = 2
      DB(1) = DIST(1)
      IF (NJ.EQ.1) DB(2) = DIST(NCHANN) + OFTEN
      DO 920 I=1,NCHANN
      IF (DIST(I).GE.DB(IJ)) IJ = IJ + 1
      IF (IJ.EQ.NJ) DB(NJ+1) = DIST(NCHANN) + OFTEN
  920 BACK2(I) = BACK(IJ-1)
      WRITE(6,930)
  930 FORMAT(13H0     DISTANCE,17X11H BACKGROUND)
      DO 940 I=1,NJ
      DIX = DB(I+1) - OFTEN
  940 WRITE(6,950) (DB(I),DIX,BACK(I))
  950 FORMAT(F8.3,14H-,F8.3,14XF6.2)
 1000 RETURN
      END
      SUBROUTINE LSQPOL(MSUB,MSUC)
      LEAST SQUARE POLYNOMIAL FIT
      COMMON /B32/ X(32), Y(32), W(50), B(10), A(10,10), XPOWER(50),
     1  DUMMY(4049)
      N=MSUB
      M=MSUB
```

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```
      M1=M+1
      M2=M+M+M
      M21=M2-1
      M41=M21+M

      FORMATION AND INVERSION OF SYSTEM OF NORMAL EQUATIONS

      DO 100 K2=M1,M41
      XPOWER(K2)=0.0
  100 CONTINUE
      DO 200 K1=1,N
      TERM=W(K1)
      DO 200 K2=M1,M21
      XPOWER(K2)=TERM+XPOWER(K2)
      TERM=X(K1)*TERM
  200 CONTINUE
      DO 300 I=1,M
      DO 300 J=1,M
      K2=I+J+M-1
      A(I,J)=XPOWER(K2)
  300 CONTINUE
      DO 400 K=1,N
      TERM=W(K)*Y(K)
      DO 400 K2=M2,M41
      XPOWER(K2)=TERM+XPOWER(K2)
      TERM=X(K)*TERM
  400 CONTINUE
      DO 500 I=1,M
      K2=I+M21
      B(I)=XPOWER(K2)
  500 CONTINUE
      CALL MATINV(A,M,B,1,DETERM,10)
  700 CONTINUE
      RETURN
      END
      SUBROUTINE PREPIP
      ...CONVERTS DATA TO CHANNEL NUMBERS AND PREPARES IT FOR THE
        VARIABLE-METRIC PACKAGE...
      REAL LPF
      COMMON /A00/ HH(20,20),PER(20),GR(20),S(20),XP(20),GP(20),T(20),
     1  G2(20),F0,GS,EL,SL,FP,GSP,T0,ZZZ,O,AA,GSC,F0,GTP,FB,GTT,GSR,
     2  DELTA,EE,LF,IS,IT,L,IHOLD(20),NSSW1,NSSW2
      COMMON/A01/Z(2100,20),SS(2102),IZSTRT(20),IZSTOP(20),P(2102),
     1  X(2100),W(2100),F(2100),G(20,20), A(20), G(20), ERR(20), DEL,
     2  DEP, F, FREST, LPF(22), LP(22), IRS, IPR, IPRF, I10, ITC, IOFF
      COMMON /A02/ STGMA(20), ERRZ(20), PERSTD(21), STORM1(20),
     1  YINTIS(20), INDEX(20), INITAL(20), IFINAL(20), STORV1(2100),
     2  DANY(2100), ITIMES, NNY
      COMMON /A03/ DUMMY(63),NB,NCALC,IGS,LQ
      COMMON /A04/ INTREF(20,10),STOREF(2100),DELTA1,DELTA2,DELTA3,
     1  STOIPR, DEFMAX, ID1, ID2, IDT, NB, NE, NREF
      COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, OFTEN.
```


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```
     1  SKIP(7),MAXREF,MAXP2
        DEL = 0.1
        DD = DIST(1)
           ...CONVERT ALL UNITS TO CHANNEL NUMBER...
        DO 1060 I=1,NT
        PERSTO(I)=(PERSTO(I)-DD)/DSTEN + 1.0
 1060 STORHH(I) = 1.0
        PERSTO  (NT+1)=9999.0
        DELT  =AINT(DELTA1+DELTA2+0.1)
        IPR=(2.0+DELTA2)
        IPRE=((2.0+DELTA2)-FLOAT(IPR))*10.0
        DO 1061 I = 1,MAXP2
 1061 B(I)=0.0
        DO 1065 I=1,IDT
 1065 B(I+1) = STOREE(I)
        IDT = IDT + 1
        I10=1
        ITIMES=0
        III = 1
           III = (NUMBER OF PEAKS ALREADY ANALYZED) + 1
 2000 IOFF = III - 1
           ...DIVIDE GROUP OF PEAKS INTO NON-OVERLAPPING SUBGROUPS...
        MS=0
        LT=0
        IF(III-NT)2001,2001,3000
           I10SS = (FIRST CHANNEL NUMBER OF FIRST PEAK IN SUBGROUP) - 1
 2001 I10SS = PERSTO(III) - DELTA2 + 0.1
        IF(I10SS.GT.1) I10SS = I10SS - 1
        DO 2015 JJ=1,20
        LT=LT+1
        IF(PERSTO  (III+JJ)-PERSTO  (III+JJ-1)- DEL3)  2015,2015,2020
 2015 CONTINUE
 2020 XXX = PERSTO(III)
           ITO = TOTAL NUMBER OF CHANNELS IN THE SUBGROUP
        ITO = PERSTO(LT+IOFF) - XXX + DELTA1 + DELTA2 + 3.1
           ...SETUP INITIAL MATRIX, DATA, WEIGHTS, AND PARAMETERS...
        DO 2025 I=1,LT
        DO 2025 J=1,LT
 2025 HH(I,J)=0.0
        DELTA=1.0
        DO 2030 I=1,LT
        IM = IOFF + I
        REF(I) = PERSTO(IM) - XXX + DELTA2 + 2.
        HH(I,I)=STORHH (IM)**2
        IF (IHOLD(IM)) 2028,2028,2027
 2027 HH(I,I) = 0.0
        GO TO 2030
 2028 DELTA = DELTA*HH(I,I)
 2030 CONTINUE
        DO 2035 I=I10,ITO
        JJ = I + I10SS - 1
        X(I)=RAWX(JJ)
```

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```
2035 W(I)=1.0/SQRT(X(I)+10.0)
     FF = FLOAT(ITC-LT)*0.05
     CALL DAVION
     ITIMES=ITIMES+1
        INDEX = NUMBER OF PEAKS IN SUBGROUP
        INITAL = STARTING CHANNEL NUMBER IN SUBGROUP
        IFINAL = FINAL CHANNEL NUMBER FOR SUBGROUP
     INDEX(ITIMES)=LT
     INITAL(ITIMES) = I10SS
     IFINAL(ITIMES) = I10SS + ITC - 1
     Q3 = ITC - LT
     ...CALC. ERRORS IN POSITIONS AND COMPUTE NORMALIZED INDIV. PEAKS
     DO 2042 I=1,LT
     IM = IOFF + I
     PERSTO  (IM)=(PER(I)+XXY-DELTA2-3.0)*OFTEN + QQ
     STORHH(IM)=HH(I,I)
     SIGMA(IM)=SQRT (ABS ((2.0*STORHH (IM)*FREST)/Q3))*OFTEN
     IF(A(I)) 2115,2110,2115
2110 ERR(IM) = 0.0
     GO TO 2120
2115 ERR(IM)=ERR(I) /A(I)
2120 DO 2040 J=1,MAXP2
2040 Z(I,IM) = Z(J,IM)*A(I)
2042 CONTINUE
     IF (IT.GE.25) WRITE(6,1001) (PERSTO(I),I=1,LT)
     III = III + LT
     GO TO 2000
3000 RETURN
1001 FORMAT(5140 EPSILON TOO SMALL - CANNOT CONVERGE FOR PEAKS AT ,5F10
    1.2/(10F10.2))
     END
     SUBROUTINE ORDER
     COMMON /A000/ HH(20,20),PER(20),GR(20),S(20),XP(20),GP(20),T(20),
    1  GR(20),F,GR,EL,SL,FR,GSR,T1,Z,C,A,GSS,FQ,GTP,FR,GTT,GSS,
    2  DELTA,F,N,MS,IT,L,IHOLD(20),NSSW1,NSSW2
     JC = N - 1
     DO 100 I=1,JC
     K = I + 1
     DO 100 J=K,N
     IF (PER(I)-PER(J)) 100,100,60
  60 SAVE = PER(I)
     PER(I) = PER(J)
     PER(J) = SAVE
     SAVE = HH(I,I)
     HH(I,I) = HH(J,J)
     HH(J,J) = SAVE
     ISAV = IHOLD(I)
     IHOLD(I) = IHOLD(J)
     IHOLD(J) = ISAV
 100 CONTINUE
     RETURN
     END
```

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```
      SUBROUTINE FUN(LLTT,GR,EC,PER,M1)
      ...SETS UP THE LINEAR EQUATIONS AND OBTAINS RELATIVE PEAK HEIGHTS.
      REAL LPF
      DIMENSION PER(21),GR(21)
      COMMON/A01/Z(2100,20),SS(2102),IZSTRT(20),IZSTOP(20),R(2102),
     1  Y(2100),W(2100),E(2100),C(20,20), A(20), G(20), ERR(20), DEL,
     2  PEP, F, FREST, LPF(22), LP(22), IRS, IPR, IPRE, I1C, ITC, IOFF
      COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, DFTEN,
     1  IDFTEN, NCHANN, II, IJ, ISPECT, IFMT, IERR,MAXREF,MAXP2
      LT=LLTT
      IF(M1.EQ.1) FREST = 1.0E10
 4006 DO 91 L=1,LT
      LP(L) = PER(L)
      LPF(L) = (PER(L)-FLOAT(LP(L)))*10.0
   91 CALL SHIFT(L)
  205 IF (M1-3) 220,210,220
      DUMMY CALL TO FUN TO FORM THE ARRAY E
  210 CALL FUN(LT)
      DO 220 I=I1C,ITC
  220 W(I) = 1.0/SQRT(ABS(E(I))+10.)
  222 DO 210 M=1,LT
      MM = M + IOFF
      DO 210 L =1,M
      LL = L + IOFF
      C(M,L) = 0.0
      DO 200 I=I1C,ITC
      IF ((I.LT.IZSTRT(LL)).OR.(I.GT.IZSTOP(LL))) GO TO 200
      IF ((I.LT.IZSTRT(MM)).OR.(I.GT.IZSTOP(MM))) GO TO 200
      IL = I - IZSTRT(LL) + 1
      IM = I -IZSTRT(MM) + 1
      C(M,L) = C(M,L) + W(I)*W(I)*Z(IL,LL)*Z(IM,MM)
  200 CONTINUE
  210 C(L,M) = C(M,L)
      DO 201 M=1,LT
      MM = M + IOFF
      A(M) = 0.0
      DO 201 I=I1C,ITC
      IF ((I.LT.IZSTRT(MM)).OR.(I.GT.IZSTOP(MM))) GO TO 201
      IM = I - IZSTRT(MM) + 1
      A(M) = A(M) + W(I)*W(I)*Y(I)*Z(IM,MM)
  201 CONTINUE
      CALL MATINV(C,LT,A,1,DETERM,ZJ)
      CALL DERIVP(LT,PER)
      DO 1600 L=1,LT
 1600 GR(L) = G(L)
      CALL FUN(LT)
      IF(M1-3) 206,1011,206
 1011 EF = F/(ITC-I1C-LT)
      DO 1006 L=1,LT
      PEP = EF*C(L,L)
 1006 ERR(L) = SQRT(ABS(PEP))
```

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```
206 FO = F
    IF (FO.LT.FBEST) FBEST = FO
    RETURN
    END
    SUBROUTINE DERIVP(LLTT,DER)
    ...CALCULATES DERIVATIVES OF FUNCTION F(FUN) WITH CHANGE
    IN POSITION
    REAL LDF
    DIMENSION DER(20)
    COMMON/A01/Z(2102,20),SS(2102),IZSTRT(20),IZSTOP(20),R(2102),
   1  X(2100),W(2100),T(2100),C(20,20), A(20), G(20), ERR(20), DEL,
   2  DER, F, FBEST, LDF(22), LP(22), IPS, IPR, IPDF, I1C, ITC, IOFF
    COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, OFTEN,
   1  NOFTEN, NCHANN, II, IJ, ISPECT, IFMT, IEPR,MAXREF,MAXP2
    LT=LLTT
    DO 95 L=1,LT
    LL = L + IOFF
    DO 94 I=1,MAXP2
 94 SS(I) = Z(I,LL)
    ISAV1 = IZSTRT(LL)
    ISAV2 = IZSTOP(LL)
    LOP=LP(L)
    LOPF=LDF(L)
    Y=DER(L)+DEL
    LP(21) = Y
    LDF(21) = (Y-FLOAT(LP(21)))*10.0
    Y=DER(L)-DEL
    LP(22) = Y
    LDF(22) = (Y-FLOAT(LP(22)))*10.0
    LP(L)=LP(21)
    LDF(L)=LDF(21)
    CALL SHIFT(L)
    CALL FUN(LT)
    FO=F
    LP(L)=LP(22)
    LDF(L)=LDF(22)
    CALL SHIFT(L)
    CALL FUN(LT)
    G(L)=(FO-F)/(2.0*DEL)
    DO 95 I=1,MAXP2
 95 Z(I,LL) = SS(I)
    IZSTRT(LL) = ISAV1
    IZSTOP(LL) = ISAV2
    LP(L)=LOP
 95 LDF(L)=LOPF
    RETURN
    END
    SUBROUTINE SHIFT(LP)
    ...CONTROLS INTERPOLATION OF ERF. PEAK FOR SHIFTING FRACTIONS
    OF CHANNELS
```


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```
      REAL LPF
      COMMON/AC1/Z(2100,20),SS(21,2),IZSTRT(20),IZSTOP(20),R(2100),
     1  X(2100),W(2100),F(2100),C(20,20), A(20), G(20), ERR(20), DEL,
     2  IRR, F, FREQ, LPF(22), LP(22), IRC, IPP, IPPF, I1C, ITC, IOFF
      COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, OFTEN,
     1  NOFTEN, NOMAIN, II, IJ, ISPECT, IFMT, TERR,MAXPEF,MAXP2
      L=L1
      LL = L + IOFF
      DO 100 J=1,MAXP2
      C1=LP(L)
      C2=LPF(L)
      U=C1+C2/10.0
      B8=IPP
      B9=IPPF
  100 Z(J,LL) = 0.0
      B1=B8+B9/10.0
      IF (B1-U) 300,13,9
      SUBROUTINE SHIFTL L LESS THAN R
    9 J=1
      IZSTRT(LL) = 1
      IF (IPPF-LPF(L)) 10,11,12
   10 F = 10+IPPF-LPF(L)
      I = IPP-LP(L)
      GO TO 14
   11 F=0.0
      GO TO 13
   12 F = IPPF-LPF(L)
   13 I = IPP-LP(L)+1
   14 F1 = F/10.0
   15 Z(J,LL) = R(I) + F1*(R(I+1)-R(I))
      I=I+1
      J=J+1
      IF (I-IPS) 16,16,17
   16 IF (J-ITC) 15,15,17
   17 IZSTOP(LL) = J - 1
      GO TO 23
      SUBROUTINE SHIFTO L EQUAL R
   18 DO 20 J=1,IPS
   20 Z(J,LL) = R(J)
      IZSTRT(LL) = 1
      IZSTOP(LL) = IPS
      GO TO 23
      SUBROUTINE SHIFTR R LESS THAN L
  300 I=1
      IF (IPPF-LPF(L)) 1,2,3
    1 F = 10+IPPF-LPF(L)
      K = LP(L)-IPP+2
      GO TO 5
    2 F=0.0
      GO TO 4
    3 F = IPPF-LPF(L)
```

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```
    4 K =LP(L)-IPP+1
    5 F1 = F/10.0
      IZSTRT(LL) = K
      J = 1
    6 Z(J,LL) = P(I) + F1*(P(I+1)-P(I))
      I=I+1
      J=J+1
      K = K + 1
      IF (I-IRS) 7,7,8
    7 IF (K-ITC) 6,6,8
    8 IZSTOP(LL) = K - 1
   23 RETURN
      END
      SUBROUTINE FUN(LT)
      ...CALCULATES THE FUNCTION F WHICH IS BEING MINIMIZED...
      REAL LPF
      COMMON/ADJ/Z(2100,20),SS(2100),IZSTRT(20),IZSTOP(20),P(2100),
     1  X(2100),W(2100),E(2100),C(20,20), A(20), G(20), ERR(20), DEL,
     2  DEP, F, FBEST, LPF(22), LP(22), IRS, IPP, IPPE, ITC, ITC, IOFF
      COMMON /DATA/ DIST(2100), COUNTS(2100), RUNID, TODAY, FREQ, OFTEN,
     1  NOFTEN, NCHAIN, II, IJ, ISPECT, IFMT, IERR,MAXREF,MAXP2
      F=0.0
      DO 60 I=1,ITC
   60 E(I) = 0.0
      DO 70 L=1,LT
      I1 = IZSTRT(L+IOFF)
      I2 = IZSTOP (L+IOFF)
      DO 70 I=I1,I2
      J = I - I1 + 1
   70 E(I) = E(I) + A(L)*Z(J,L+IOFF)
      DO 80 I=I1C,ITC
      F1 = (X(I)-E(I))*W(I)
   80 F = F + F1*F1
      RETURN
      END
      SUBROUTINE MATINV(A,NSUB,B,MSUB,DET,NMAX)

      DIMENSION A(NMAX,NSUB),B(NMAX,MSUB)
      DIMENSION PIVOT(100),INDEX(100),IPIVOT(100)
      EQUIVALENCE (PIVOT,INDEX,IPIVOT),(AMAX,T),(IROW,I1,IRC),
     1            (TEMP,SWAP)
      DATA (ISHIFT=4036),(MASK=00000077777778)

      N=NSUB
      M=MSUB

      INITIALIZATION

      DETERM=1.0
      DO 20 I=1,N
      IPIVOT(I)=0
```

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```
 20 CONTINUE
    DO 550 I=1,N

    SEARCH FOR PIVOT ELEMENT

    AMAX=0.
    DO 105 J=1,N
    TEMP=IPIVOT(J).AND..NOT.MASK
    IF(TEMP) 105,60
 60 DO 100 K=1,N
    TEMP=IPIVOT(K).AND..NOT.MASK
    IF(TEMP) 100,80
 80 TEMP=ABS (A(J,K))
    IF(TEMP-AMAX) 100,85,85
 85 IROW=J.
    ICOLUM=K
    AMAX=TEMP
100 CONTINUE
105 CONTINUE
    INDEX(I)=INDEX(I)+(ICHIFT*IROW+ICOLUM)
    J=IROW
    AMAX=A(J,ICOLUM)
    DETERM=AMAX*DETERM

    MATRIX SINGULAR

    IF(DETERM) 110,500

110 PIVOT(ICOLUM)=INDEX(ICOLUM).OR.AMAX.AND..NOT.MASK

    INTERCHANGE ROWS

    IF(IROW-ICOLUM) 140,260
140 DETERM=-DETERM
    DO 200 K=1,N
    SWAP = A(J,K)
    A(J,K)=A(ICOLUM,K)
    A(ICOLUM,K)=SWAP
200 CONTINUE
    DO 250 K=1,M
    SWAP=B(J,K)
    B(J,K)=B(ICOLUM,K)
    B(ICOLUM,K)=SWAP
250 CONTINUE

    DIVIDE PIVOT ROW

260 K=ICOLUM
    A(ICOLUM,K)=1.
    DO 350 K=1,N
    A(ICOLUM,K)=A(ICOLUM,K)/AMAX
```

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```
  350 CONTINUE
      DO 370 K=1,M
      B(ICOLUM,K)=B(ICOLUM,K)/AMAX
  370 CONTINUE

      REDUCE

      DO 550 J=1,N
      IF(J-ICOLUM)400,550
  400 T=A(J,ICOLUM)
      A(J,ICOLUM)=0.0
      DO 450 K=1,N
      A(J,K)=A(J,K)-A(ICOLUM,K)*T
  450 CONTINUE
      DO 500 K=1,M
      B(J,K)=B(J,K)-B(ICOLUM,K)*T
  500 CONTINUE
  550 CONTINUE

      INTERCHANGE

  600 DO 710 I=1,N
      I1=N+1-I
      IRC=INDEX(I1).AND.MASK
      K=IRC/ISHIFT
      ICOLUM=IRC-K*ISHIFT
      IF(K-ICOLUM) 650,710
  650 DO 705 J=1,N
      SWAP=A(J,K)
      A(J,K)=A(J,ICOLUM)
      A(J,ICOLUM)=SWAP
  705 CONTINUE
  710 CONTINUE

  740 DET=DETERM
      RETURN
      ENTRY OMATINV
      RETURN
      END
      SUBROUTINE DAVION
      ...THIS IS THE CONTROL ROUTINE FOR THE VARIABLE-METRIC PACKAGE...
      COMMON /A00/ H(20,20),X(20),G(20),S(20),XP(20),GP(20),T(20),
     1  G3(20),F,GS,FL,DL,FP,GSP,TO,Z,C,A,GSS,F0,GTP,F8,GTI,GSP,
     2  DELTA,E,N,MS,IT,L,IHOLD(20),NSSW1,NSSW2
   15 M1=1
      IT = 0
      E=2.0
      CALL FCN(N,G,F,Y,M1)
      IF(NSSW1)20,25,20
   20 WRITE(6,8) IT,MS,F
      GO TO 840
```

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```
  120 M1=2
  200 CALL READY
      GO TO (300,300,500,500), L
  300 CALL AIM
      GO TO (400,500,500,500), L
  400 CALL FIRE
      GO TO (500,500,300,300), L
  500 CALL PROCESS
      IF (IT-25) 120,800,550
  550 M1 = 3
      GO TO 900
  800 M1=2
      IF(NSSW1)22,25,22
   22 WRITE(6,11)
  810 DO 820 II=1,N
  820 WRITE(6,7) (H(II,JJ),JJ=1,N)
  830 WRITE(6,12) DELTA,E,GS
  840 IF(NSSW1)24,25,24
   24 WRITE(6,13) (X(I),I=1,N)
      GO TO (850,850,860), M1
  850 WRITE(6,13) (G(I),I=1,N)
  860 WRITE(6,9)
   25 GO TO (120,120,900), M1
  900 IF (N.GT.1) CALL ORDER
      CALL FCN(N,G,E,X,M1)
   30 RETURN
    3 FORMAT(9E12.5)
    7 FORMAT(1H 8E14.5)
    8 FORMAT(4H0IT I4,7H  STEP I4,4H  E=E14.5)
    9 FORMAT(20H0- - - - - - - - - -)
   10 FORMAT(3H0X=8E14.5/(3H0  8E14.5))
   11 FORMAT(17H0ETNAL VALUES/13H0ERROR MATRIX)
   12 FORMAT(7H0DELTA=E14.5,4H  E=E14.5,6H  GS=E14.5)
   13 FORMAT(3H0G=8E14.5/(3H0  8E14.5))
      END
      SUBROUTINE READY
      COMMON /100/ H(20,20),X(20),G(20),S(20),XP(20),GP(20),T(20),
     1  B3(20),E,GS,EL,SL,EB,GSB,TO,Z,O,A,GSS,EO,GTP,EB,GTT,GSB,
     2  DELTA,E,N,MS,IT,L,IHOLD(20),NSSW1,NSSW2
  200 L=1
      CALL MATMPY(N,N,H,G,S)
      DO 205 I=1,N
  205 S(I)=-S(I)
      CALL MATMPY(1,N,S,G,GS)
      IF (GS+E) 210,240,240
  210 L=2
      EL=2.0
      TO=EL*E/GS
      IF (TO+EL) 217, 217, 212
  212 EL=-TO
  217 SL=-GS
```

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```
      DO 215 I=1,N
  215 XP(I)=X(I)+SL*S(I)
      CALL FCN(N,GP,FP,XP,2)
      CALL MATMPY(1,N,N,GP,GSP)
      IF (-GSP) 240,240,220
  220 IF (F-FP) 240,240,225
  225 L=3
      IF(NSSW1)100,101,100
  100 WRITE(6,1)
  101 FB=FP
      DO 230 I=1,N
      GB(I)=GP(I)
      T(I)=XP(I)
  230 CONTINUE
      IF (EL+2.0) 240,235,240
  235 L=4
      DELTA=DELTA+DELTA
      T0=1.0/S_
  240 RETURN
    1 FORMAT(10HUNDERSHOT)
      END
      SUBROUTINE AIM
      COMMON /A00/ H(20,20),X(20),G(20),S(20),XP(20),GP(20),T(20),
     1  GB(20),F,GS,EL,SL,FP,GSP,T0,Z,Q,A,GSS,F0,GTP,FB,GTT,GSB,
     2  DELTA,E,N,MS,IT,L,IHOLD(20),NSSW1,NSSW2
  300 L=1
      Z=2.0/EL*(F-FP)+GS+GSP
      Q=ABS (Z+SQRT (1.0-(GS/Z)*(GSP/Z)))
      A=(Q-Z+GSP)/(Q+Q-GS+GSP)
      T0=EL/3.0*(Q+Q+Z+GSP)*A**4
      F0=FP-T0
      CALL MATMPY(N,N,H,GP,T)
      DO 305 I=1,N
  305 T(I)=(GSP/SL)*S(I)-T(I)
      CALL MATMPY(1,N,T,GP,GTP)
      IF (T0+T0+GTP) 315,310,310
  310 DO 312 I=1,N
  312 T(I)=XP(I)+A*(X(I)-XP(I))
      GO TO 340
  315 IF (F+F+GTP) 310,320,320
  320 DO 322 I=1,N
  322 T(I)=T(I)+XP(I)
      CALL FCN(N,GB,FB,T,2)
      IF (F)-FB) 310,325,325
  325 L=3
      IF(NSSW1)100,101,100
  100 WRITE(6,1)
  101 DO 327 I=1,N
  327 S(I)=T(I)-XP(I)
      CALL MATMPY(1,N,S,GB,GTT)
      GTT=GTT-GTP
```

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```
      IF (GTT) 340,330,330
  330 L=2
      GSS=GTT
      SL=-GTP
      EL=1.0
  340 RETURN
    1 FORMAT(9H0PIVOT=E7.1)
      END
      SUBROUTINE STEP
      COMMON /100/ W(20,20),X(20),G(20),S(20),XP(20),GP(20),T(20),
     1  GB(20),E,GS,EL,SL,EP,GSP,TO,Z,Q,A,GSS,E0,GTP,EB,GTT,GSB,
     2  DELTA,I,N,MS,IT,L,THOLD(20),NSSW1,NSSW2
      EQUIVALENCE (TEMP,GTT)
  400 L=1
      TEMP=A/(1.0-A)
      CALL RON(N,GB,EB,T,2)
      CALL MATMPY(1,N,S,GB,GSP)
      TO=E
      IF (TO-EP) 403, 403, 402
  402 TO=EP
  403 IF (TO-EB+E) 415, 405, 405
  405 GSO=0+2
      TO=GSO*(TEMP-1.0/TEMP)
      IF (ABS (TO)-0) 430,410,410
  410 L=2
      GO TO 440
  415 L=2
      IF(EP-E) 425,420,420
  420 IF(NSSW1)100,101,100
  100 WRITE(6,1)
  101 EL=(1.0-A)*EL
      EP=EB
      GSP=GSB
      DO 422 I=1,N
      XP(I)=T(I)
      GP(I)=GB(I)
  422 CONTINUE
      GO TO 440
  425 IF(NSSW1)200,201,200
  200 WRITE(6,2)
  201 EL=EL*A
      E=EB
      GS=GSB
      DO 427 I=1,N
      X(I)=T(I)
      G(I)=GB(I)
  427 CONTINUE
      GO TO 440
  430 GSS=GSS+TO
      DO 435 I=1,N
  435 G(I)=(GB(I)-G(I))*TEMP+(GP(I)-GB(I))/TEMP
```

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```
      RETURN
    1 FORMAT(10H0MOVE LEFT)
    2 FORMAT(11H0MOVE RIGHT)
      END
      SUBROUTINE PRESS
      COMMON /AGC/ H(20,20),X(20),G(20),S(20),XP(20),GP(20),T(20),
     1  G3(20),F,GS,FL,GL,FP,GSP,T0,Z,O,A,GSS,F0,GTP,FR,GTT,GSR,
     2  DELTA,E,N,MS,IT,L,THOLD(20),NSSW1,NSSW2
  501 GO TO (505,720,730,525), L
  505 CALL MATMPY(H,N,H,G,X)
      CALL MATMPY(1,N,X,G,T0)
      IF (T0-GSS**2/GL-E) 515,510,510
  510 DO 512 II=1,N
      DO 512 JJ=1,N
  512 H(II,JJ)=H(II,JJ)-X(II)*X(JJ)/T0
      DELTA=DELTA*(FL*GSS/T0)
      T0=FL/GSS
      GO TO 525
  515 IF(NSSW1) 200,520,200
  211 WRITE(6,1)
  520 DELTA=DELTA*(FL*GL/GSS)
      T0=FL/GSS-1.0/GL
  525 DO 527 II=1,N
      DO 527 JJ=1,N
  527 H(II,JJ)=H(II,JJ)+T0*S(II)*S(JJ)
  530 IT=IT+1
      E=0.0
      IF(NSSW1)100,101,100
  100 WRITE(6,4) IT,MS,F,GS
  101 DO 532 I=1,N
      G(I)=G3(I)
      X(I)=T(I)
  532 CONTINUE
      IF(NSSW1)535,540,535
  535 WRITE(6,2) (X(I),I=1,N)
      WRITE(6,3) DELTA
  540 RETURN
    1 FORMAT(9H0COLINEAR)
    2 FORMAT(3H0X=,8E14.5/(3H0  ,8E14.5))
    3 FORMAT(7H0DELTA=,E14.5/20H0- - - - - - - - - -)
    4 FORMAT(4H0IT ,I4,7H  STEP ,I4,4H  F=,E14.5,5H  GS=,E14.5)
      END
      SUBROUTINE MATMPY(M,N,H,G,S)
      DIMENSION H(20,20),G(20),S(20)
  700 DO 720 II=1,M
      S(II)=0.0
      DO 720 JJ=1,N
  720 S(II)=H(JJ,II)*G(JJ)+S(II)
  741 RETURN
      END
```

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VITA

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER GNE/PH/78M-5	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) A COMPUTER CODE TO ANALYZE ALPHA SPECTRA		5. TYPE OF REPORT & PERIOD COVERED MS Thesis 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Richard S. Hartley 2nd Lt USAF		8. CONTRACT OR GRANT NUMBER(s)
9. PERFORMING ORGANIZATION NAME AND ADDRESS Air Force Institute of Technology (AFIT-ENP) Wright-Patterson AFB, Ohio 45433		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS McClellan Central Laboratory (MCLN) 1155th Technical Operation Squadron McClellan AFB, CA 95652		12. REPORT DATE March, 1978 13. NUMBER OF PAGES 88
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

Approved for public release; IAW AFR 190-17

JERRAL F. GUESS, Captain USAF
Director of Information

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Alpha Pulse-Height Analysis
Alpha Spectroscopy
Plutonium 239, Plutonium 240
Pulse-Height Analysis

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A computer code was modified to analyze pulse-height spectra detected by semiconductor detectors. The program fit the spectra with a reference peak which was expressed as a table of values. The results of the analysis were dependent upon reference peak chosen; hence, reference peak selection became the main emphasis. The error resulting in each analysis was greater than three standard deviations of the actual area and was suspected to have occurred because of miscalculation of the reference peak.

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